

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061820\
 Data File : BF120647.D
 Acq On : 18 Jun 2020 17:39
 Operator : JU/CG
 Sample : L3034-11
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-4

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-BF061020.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	5.416	561	566	569	rBV	2926470	2953902	75.72%	9.835%
2	6.439	734	740	743	rBV	2731974	2909146	74.57%	9.686%
3	6.798	798	801	805	rBV	1058525	831462	21.31%	2.768%
4	6.957	824	828	831	rBV	3145177	2591960	66.44%	8.630%
5	7.363	892	897	900	rBV	2394842	2076901	53.24%	6.915%
6	8.080	1015	1019	1027	rBV	1310605	1082178	27.74%	3.603%
7	9.157	1198	1202	1205	rBV	4559574	3901159	100.00%	12.988%
8	9.545	1265	1268	1273	rBV	265271	241584	6.19%	0.804%
9	9.833	1313	1317	1325	rBV	1209060	970530	24.88%	3.231%
10	10.539	1432	1437	1445	rBV9	16697	44036	1.13%	0.147%
11	10.621	1447	1451	1462	rVV	2284542	2251751	57.72%	7.497%
12	10.745	1469	1472	1479	rVB4	33864	60554	1.55%	0.202%
13	11.121	1533	1536	1540	rBV6	21450	45490	1.17%	0.151%
14	11.316	1565	1569	1573	rBV	1112658	1059897	27.17%	3.529%
15	11.592	1613	1616	1621	rVB7	24875	47317	1.21%	0.158%
16	11.845	1657	1659	1662	rBV3	57772	51461	1.32%	0.171%
17	12.910	1835	1840	1843	rVB	3738328	3830998	98.20%	12.755%
18	13.186	1885	1887	1891	rVB3	53236	59765	1.53%	0.199%
19	13.380	1917	1920	1925	rBV4	60181	79848	2.05%	0.266%
20	13.604	1956	1958	1963	rBV5	44346	46974	1.20%	0.156%
21	13.804	1989	1992	1997	rBV2	306184	455124	11.67%	1.515%
22	13.957	2014	2018	2021	rVB	1114105	962916	24.68%	3.206%
23	14.245	2065	2067	2072	rBV4	107080	135958	3.49%	0.453%
24	14.398	2092	2093	2094	rBV	160717	105342	2.70%	0.351%
25	14.915	2179	2181	2183	rVB2	73536	48155	1.23%	0.160%
26	14.974	2189	2191	2199	rBV6	127687	274485	7.04%	0.914%
27	15.162	2220	2223	2232	rBV8	123381	312098	8.00%	1.039%
28	15.398	2259	2263	2270	rBV	826794	1017627	26.09%	3.388%
29	15.498	2278	2280	2282	rBV2	128572	171544	4.40%	0.571%
30	16.051	2373	2374	2378	rBV4	105154	171919	4.41%	0.572%
31	16.127	2385	2387	2391	rBV4	86593	66651	1.71%	0.222%
32	16.274	2410	2412	2418	rBV6	94556	152268	3.90%	0.507%
33	16.421	2436	2437	2444	rBV7	90838	127416	3.27%	0.424%
34	16.539	2455	2457	2463	rBV5	95456	161236	4.13%	0.537%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.774	2493	2497	2499	rBV4	73867	124747	3.20%	0.415%
36	16.903	2518	2519	2525	rBV4	101709	144951	3.72%	0.483%
37	16.968	2529	2530	2535	rBV5	56073	77950	2.00%	0.260%
38	17.092	2550	2551	2554	rBV3	85906	67808	1.74%	0.226%
39	17.186	2564	2567	2572	rBV6	122193	320388	8.21%	1.067%

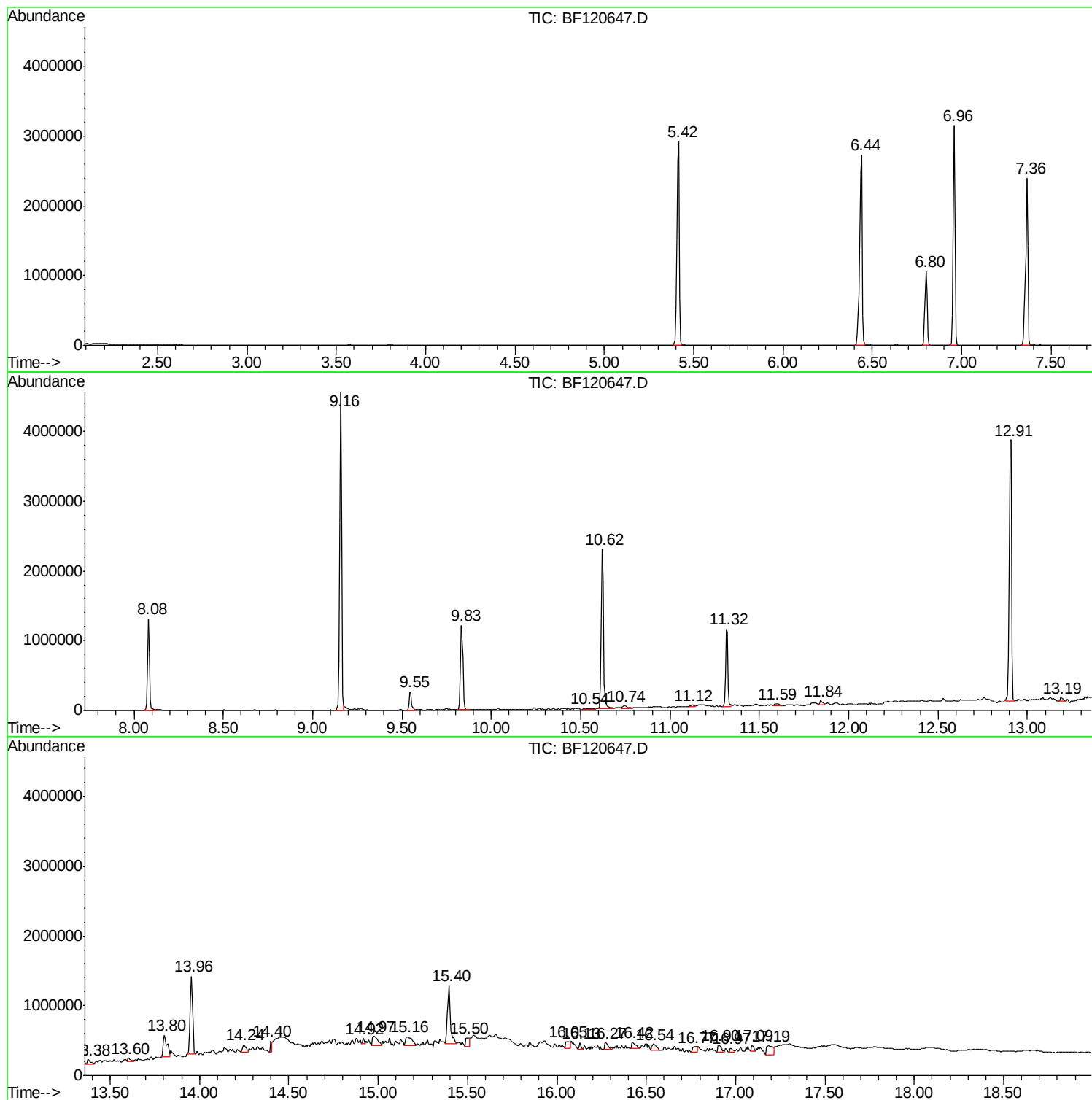
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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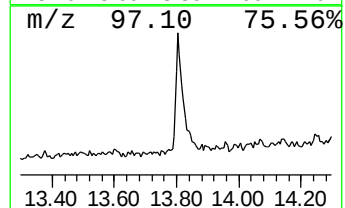
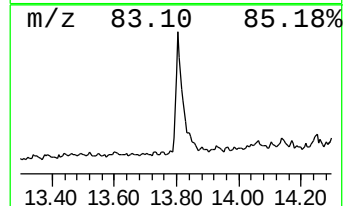
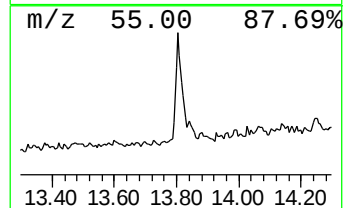
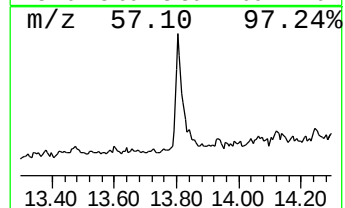
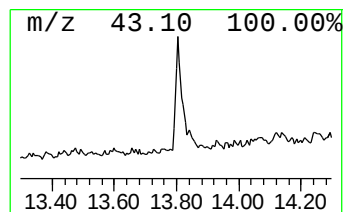
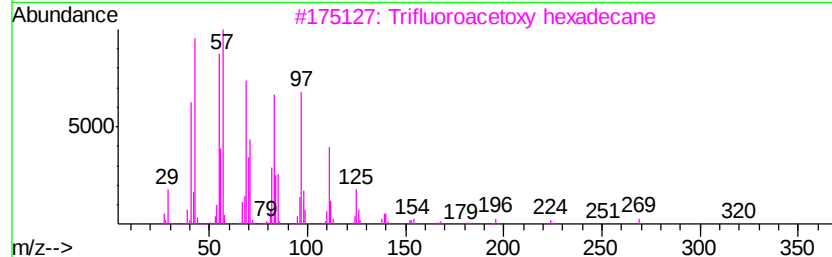
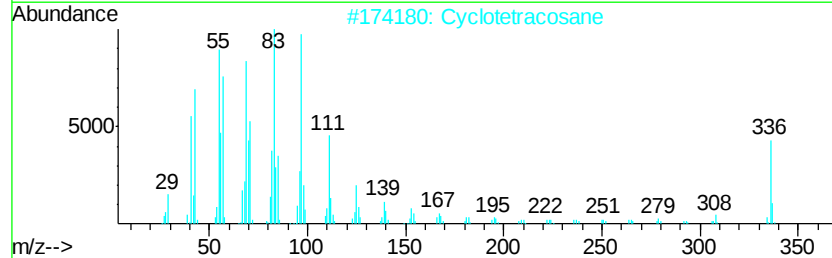
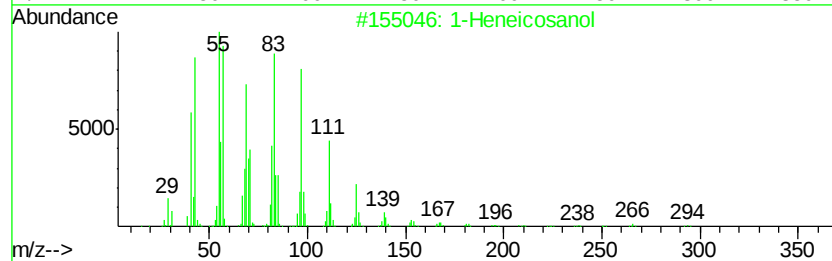
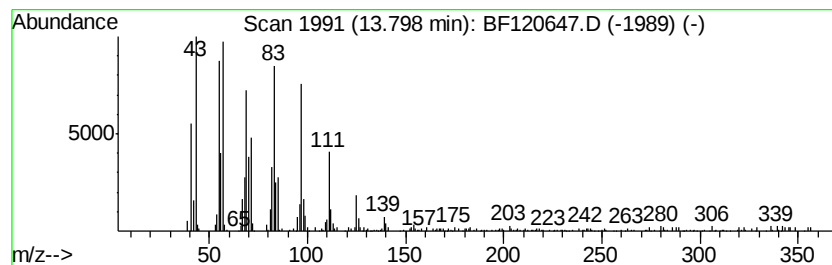
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.80	9.45 ng	455124	Chrysene-d12	13.96	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Cyclotetracosane	336	C24H48	000297-03-0	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94



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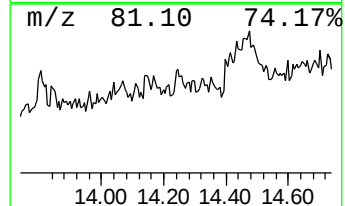
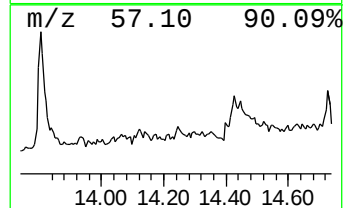
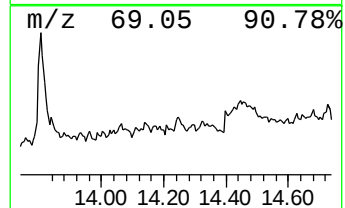
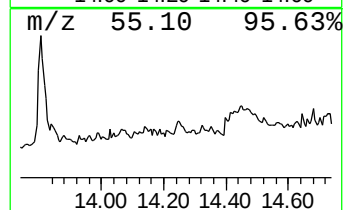
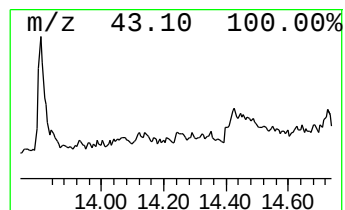
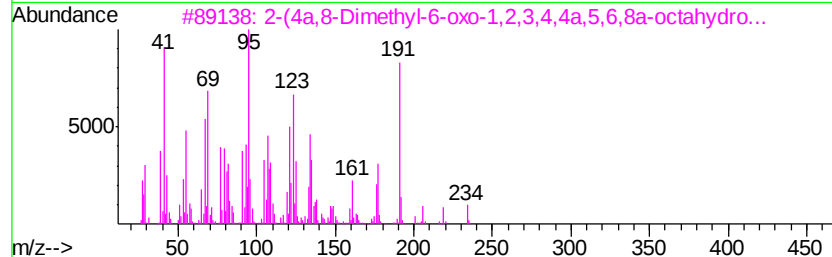
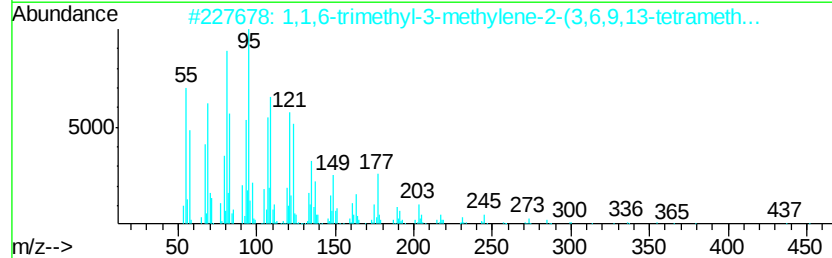
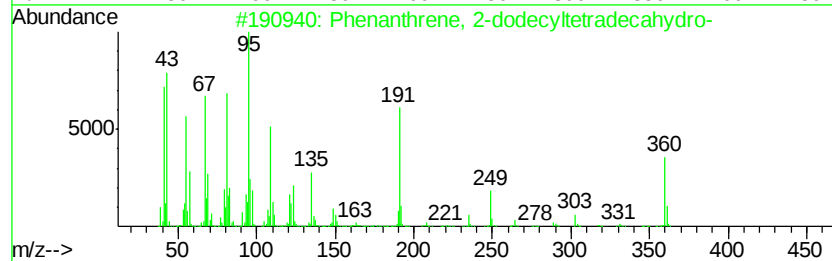
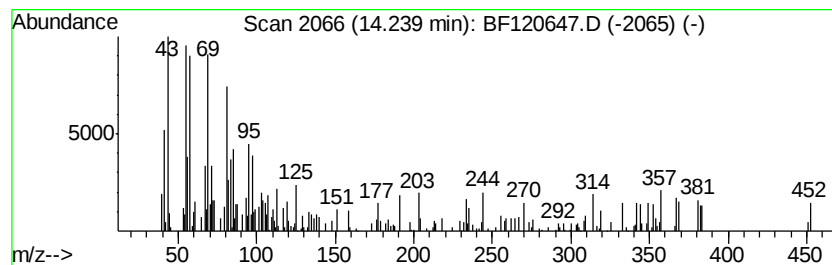
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Phenanthrene, 2-dodecyltetra... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.24	2.82 ng	135958	Chrysene-d12	13.96		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenanthrene, 2-dodecyltetradeca...	360	C26H48	055334-22-0	87
2		1,1,6-trimethyl-3-methylene-2-(3...	452	C33H56	1000373-94-5	70
3		2-(4a,8-Dimethyl-6-oxo-1,2,3,4,4...	234	C15H22O2	1000190-21-8	53
4		Pyridine, 3-(5-furan-2-yl-[1,2,4...	349	C19H15N3O4	1000316-99-5	42
5		2-Furancarboxamide, N-[1-[(2,4-d...	349	C16H13Cl2N3O2	1000350-40-2	42



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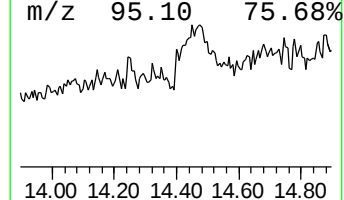
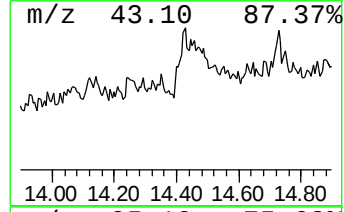
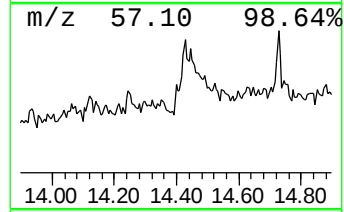
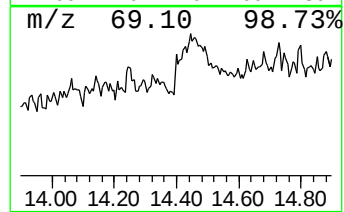
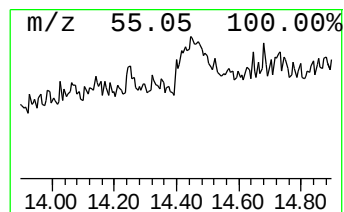
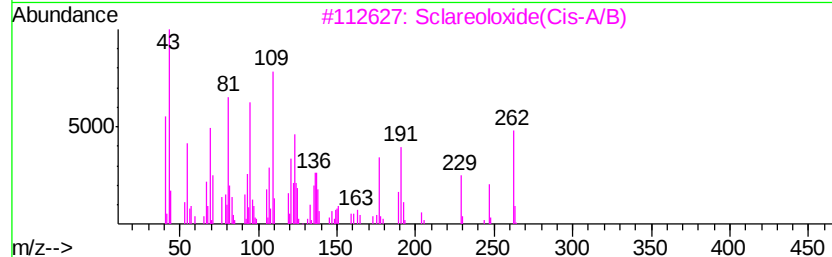
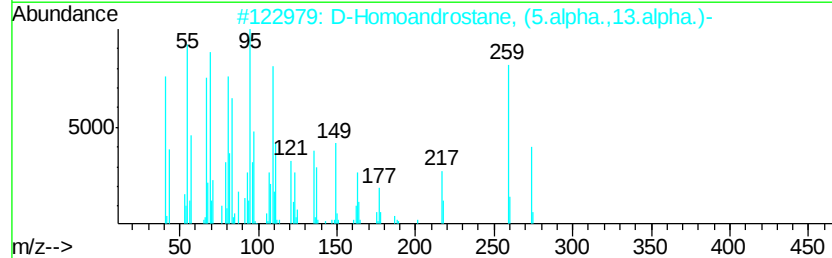
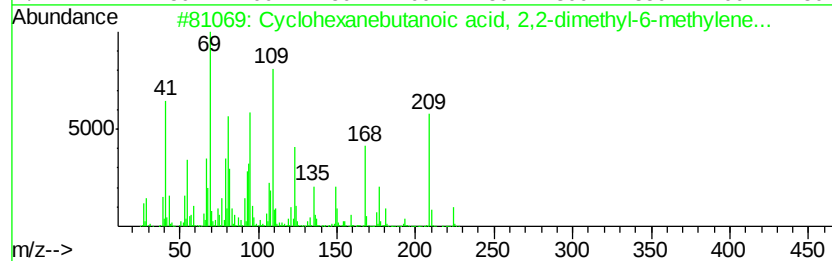
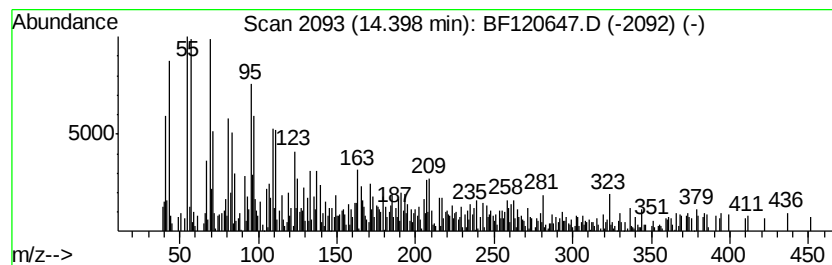
Instrument :
BNA_F
ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Cyclohexanebutanoic acid, 2... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.40	2.19 ng	105342	Chrysene-d12	13.96		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cvclohexanebutanoic acid, 2,2-di...	224	C14H24O2	095452-15-6	70
2		D-Homoandrostane, (5.alpha.,13.a...	274	C20H34	054482-31-4	49
3		Sclareoloxide(Cis-A/B)	262	C18H30O	1000215-78-3	43
4		2,2,4a,6a,8a,9,12b,14a-Octamethv...	410	C30H50	053013-35-7	42
5		8-Decenoic acid, 5-ethenyl-3,5,9...	252	C16H28O2	056114-53-5	41



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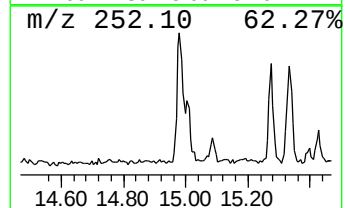
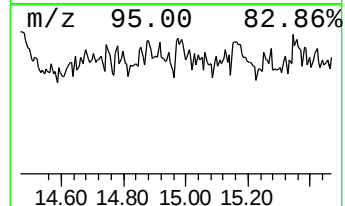
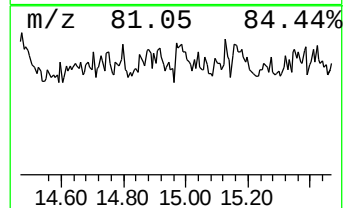
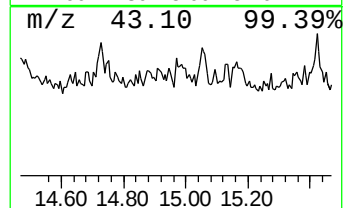
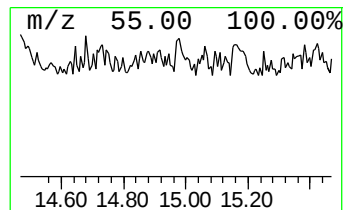
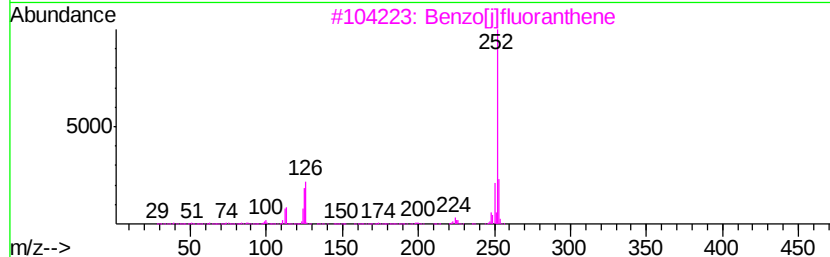
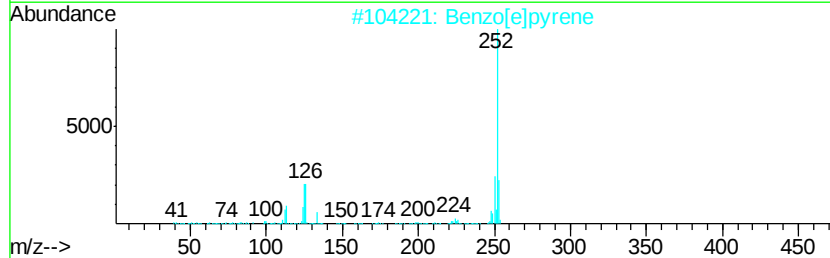
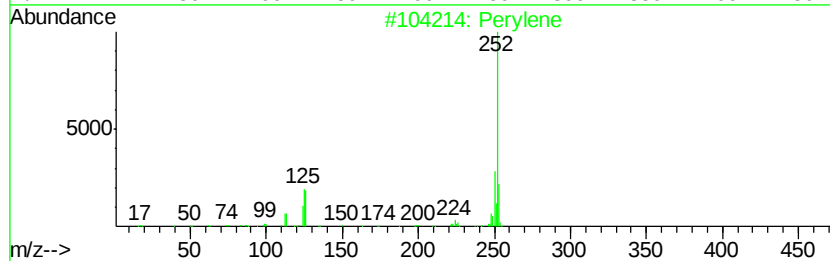
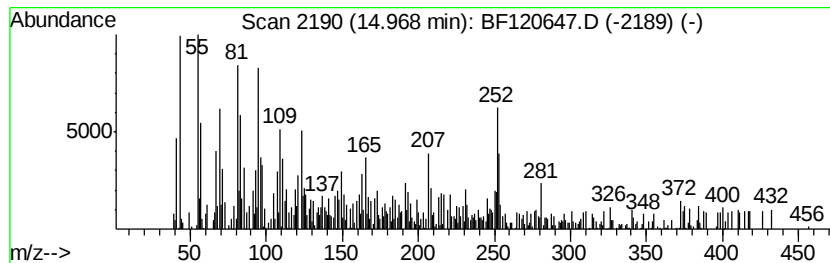
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Perylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	5.39 ng	274485	Perylene-d12	15.40

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene		252	C20H12	000198-55-0	74
2	Benzo[e]pyrene		252	C20H12	000192-97-2	55
3	Benzo[i]fluoranthene		252	C20H12	000205-82-3	42
4	Benzo[k]fluoranthene		252	C20H12	000207-08-9	38
5	Benzo[a]pyrene		252	C20H12	000050-32-8	38



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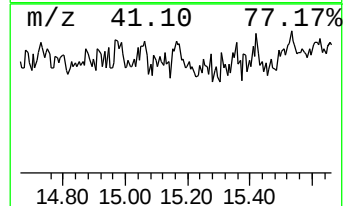
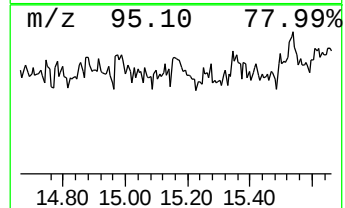
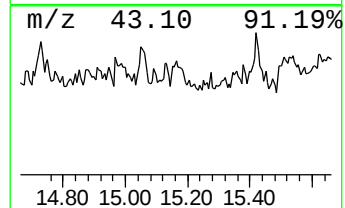
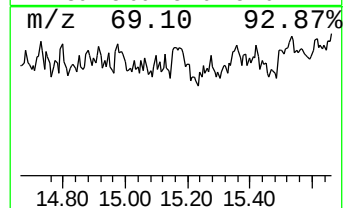
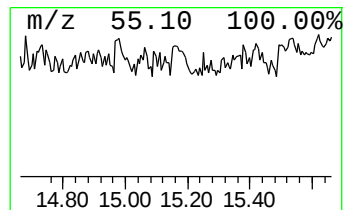
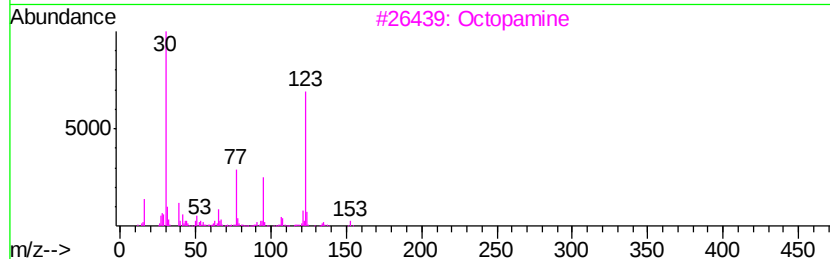
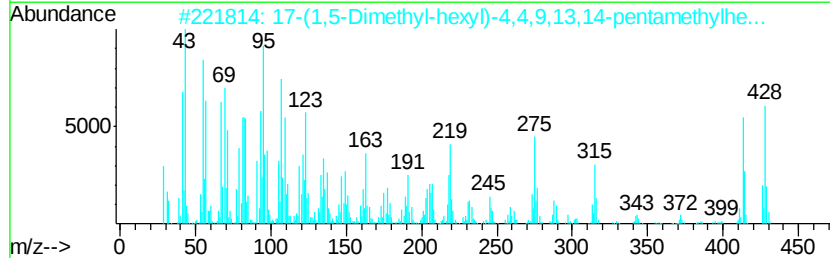
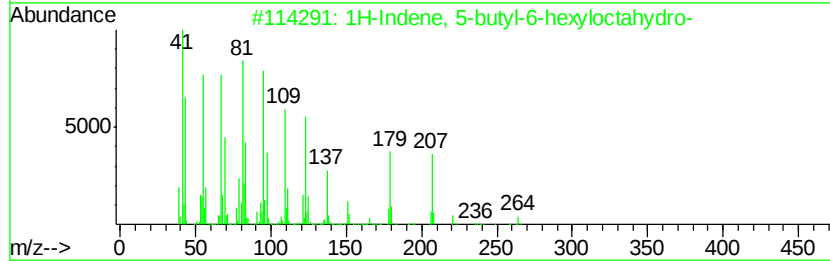
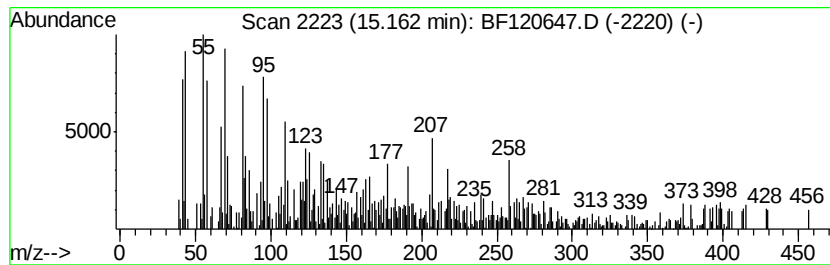
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1H-Indene, 5-butyl-6-hexylo... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.16	6.13 ng	312098	Perylene-d12		15.40
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 5-butyl-6-hexyloctahydro...	264	C19H36	055044-36-5	60
2	17-(1,5-Dimethyl-hexyl)-4,4,9,13...	428	C30H52O	1000187-63-0	49
3	Octopamine	153	C8H11NO2	000104-14-3	38
4	Piperazine, N-(2-furoyl)-N'-[2-(...	445	C22H24ClN3O3S	156483-16-8	37
5	Gorgostane, (5.alpha.)-	412	C30H52	056143-37-4	37



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061820\
Data File : BF120647.D
Acq On : 18 Jun 2020 17:39
Operator : JU/CG
Sample : L3034-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

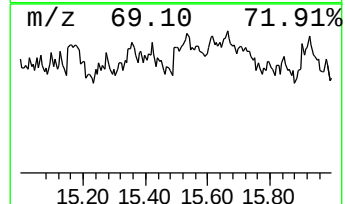
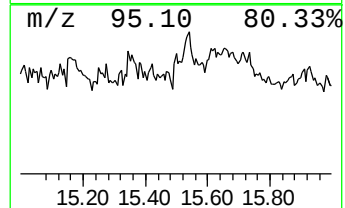
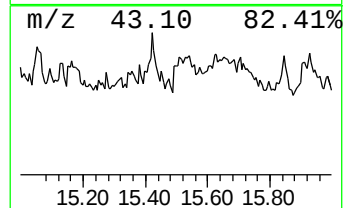
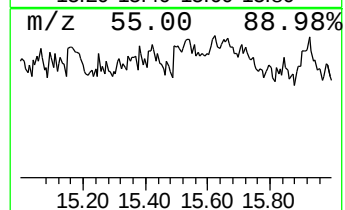
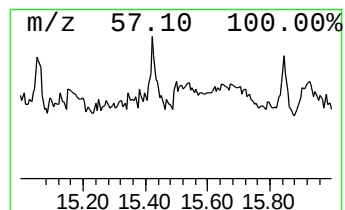
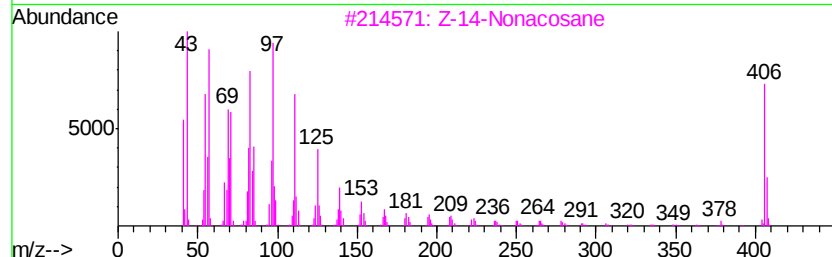
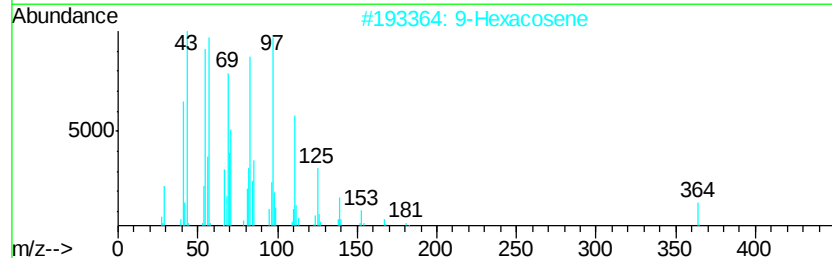
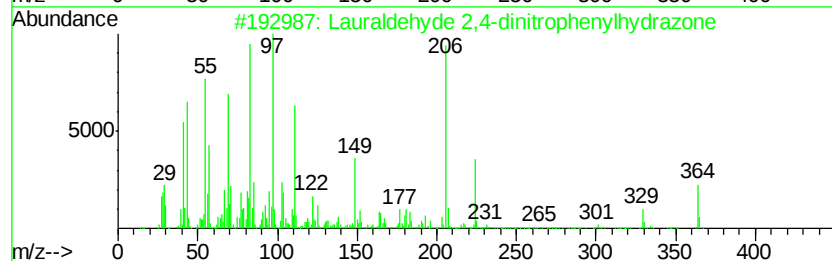
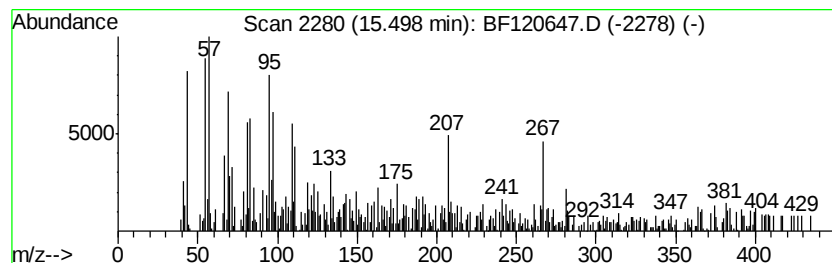
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown15.50 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.50	3.37 ng	171544	Perylene-d12	15.40

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lauraldehyd 2,4-dinitrophenylhy...	364	C18H28N4O4	001726-78-9	48
2			9-Hexacosene	364	C26H52	071502-22-2	45
3			Z-14-Nonacosane	406	C29H58	1000131-18-9	44
4			1,3-Dioxolane, 4-ethyl-5-octyl-2...	350	C15H24F6O2	038274-72-5	25
5			Cholestan-3-ol, 4,4-dimethyl-, (...)	416	C29H52O	002550-84-7	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061820\
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Misc :
ALS Vial : 7 Sample Multiplier: 1

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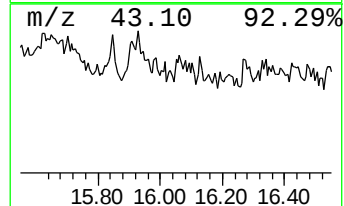
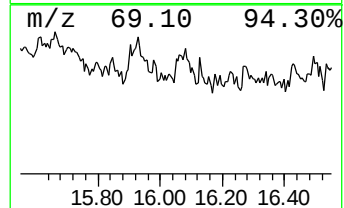
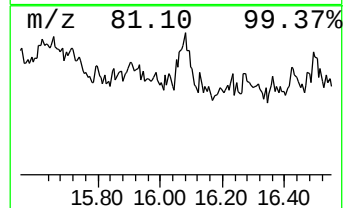
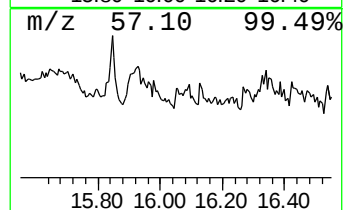
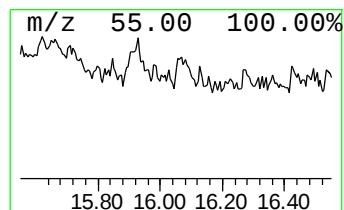
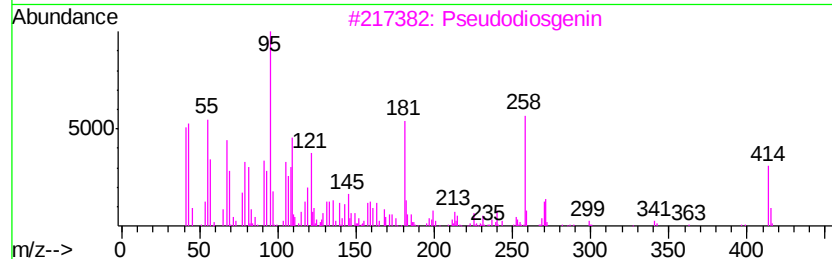
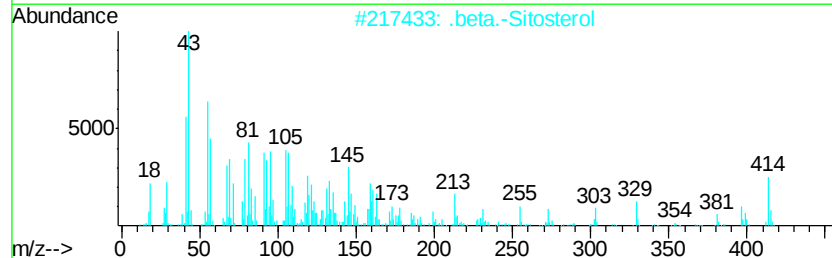
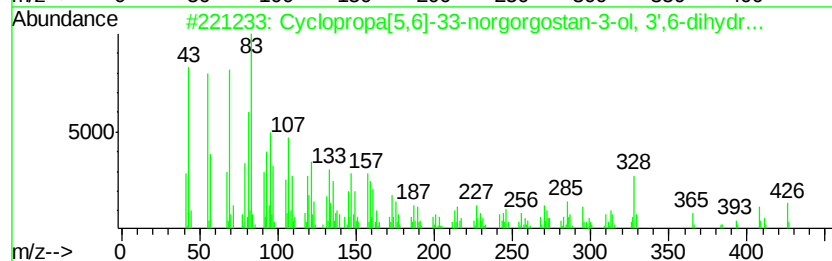
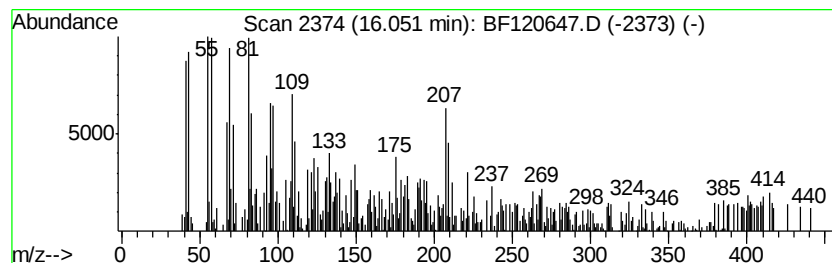
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.05 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.05	3.38 ng	171919	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopropa[5,6]-33-norgorgostan-...	426	C30H500	053761-94-7	15
2		.beta.-Sitosterol	414	C29H500	000083-46-5	11
3		Pseudodiosgenin	414	C27H4203	006808-14-6	11
4		.gamma.-Sitosterol	414	C29H500	000083-47-6	10
5		Azafrin	426	C27H3804	000507-61-9	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061820\
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Misc :
ALS Vial : 7 Sample Multiplier: 1

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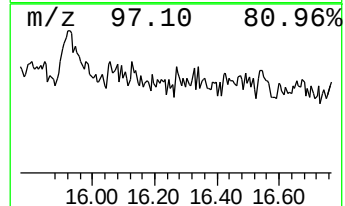
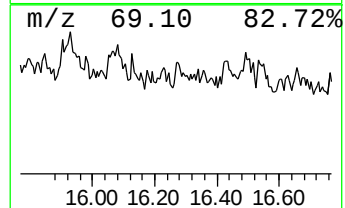
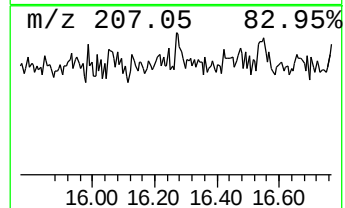
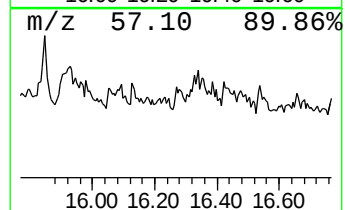
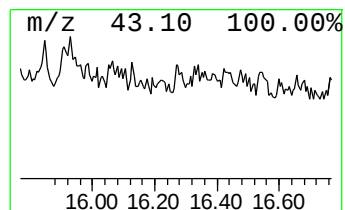
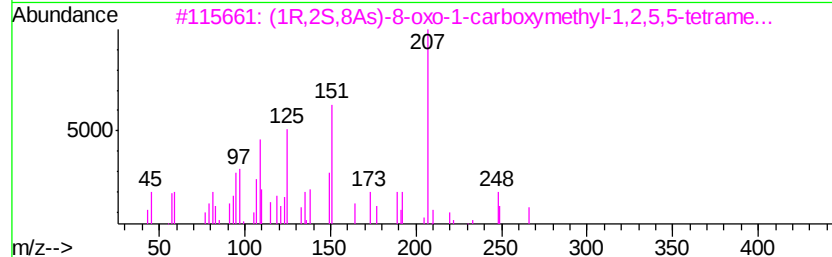
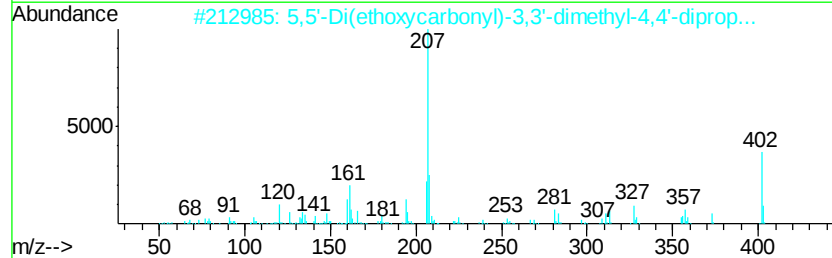
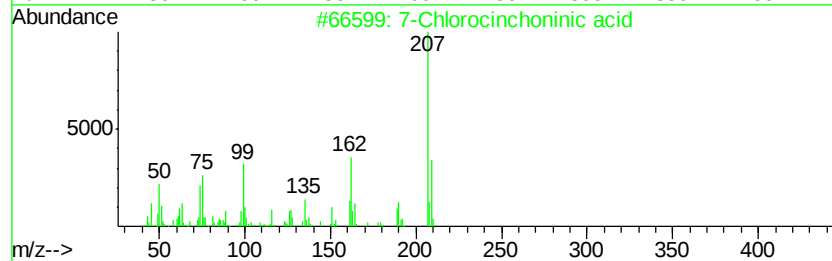
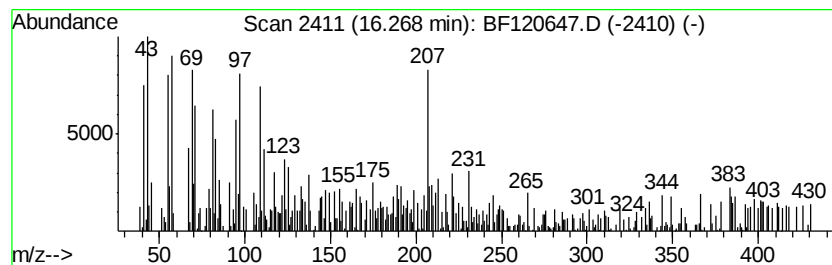
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown16.27 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.27	2.99 ng	152268	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	7-Chlorocinchoninic acid	207	C10H6ClN02	013337-66-1	35
2		5,5'-Di(ethoxycarbonyl)-3,3'-dim...	402	C23H34N2O4	102586-97-0	35
3		(1R,2S,8As)-8-oxo-1-carboxymethv...	266	C16H26O3	1000298-98-2	25
4		2H-3,9a-Methano-1-benzoxepin, oc...	222	C15H26O	005956-09-2	22
5		4-Quinolinecarboxylic acid, 2-ch...	207	C10H6ClN02	005467-57-2	20



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061820\
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Misc :
ALS Vial : 7 Sample Multiplier: 1

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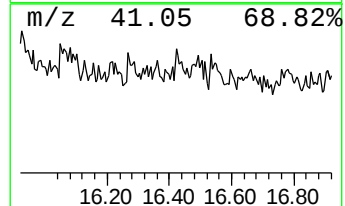
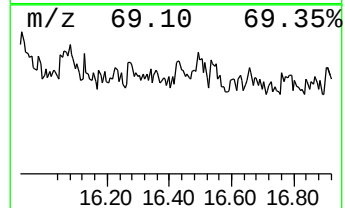
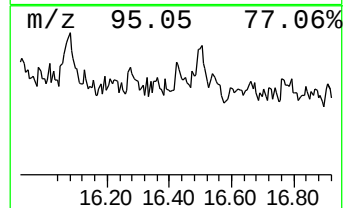
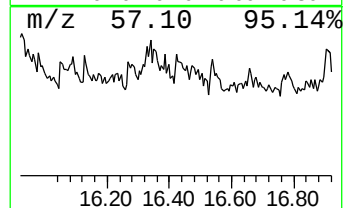
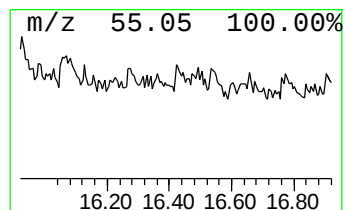
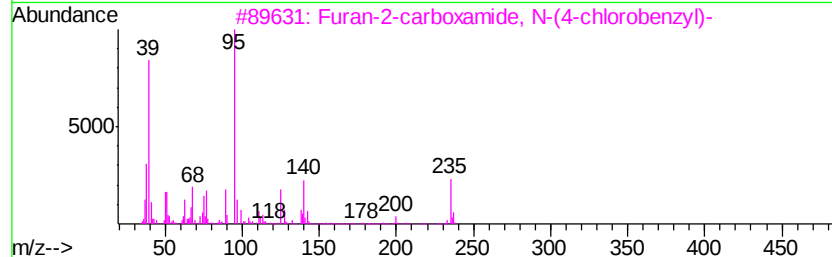
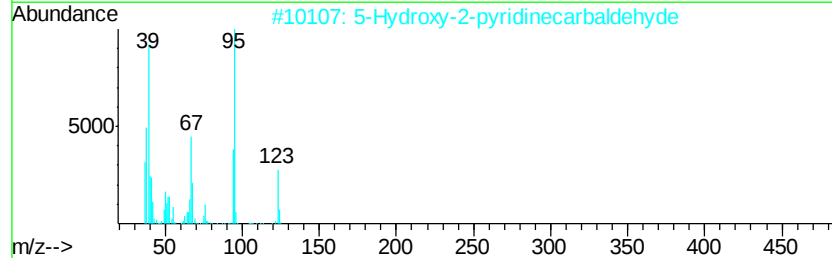
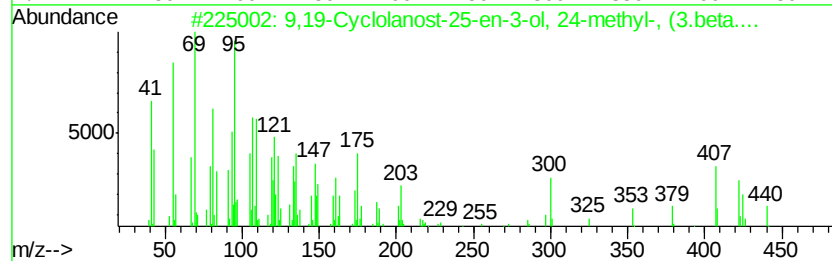
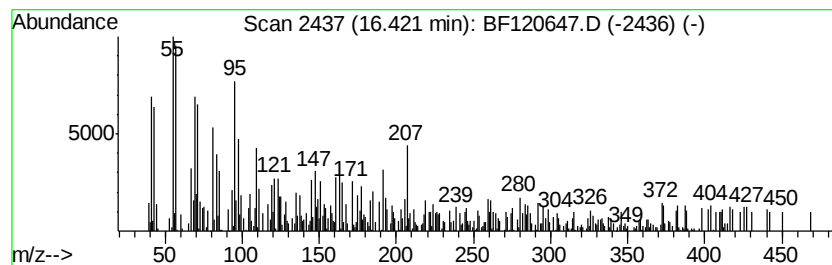
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown16.42 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.42	2.50 ng	127416	Perylene-d12	15.40

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,19-Cyclolanost-25-en-3-ol, 24-...	440	C31H52O	000511-61-5	38		
2	5-Hydroxy-2-pyridinecarbaldehyde	123	C6H5NO2	031191-08-9	35		
3	Furan-2-carboxamide, N-(4-chloro...	235	C12H10ClN02	1000259-35-4	25		
4	1H-Indene, 5-butyl-6-hexyloctahy...	264	C19H36	055044-36-5	25		
5	Cholest-4-en-3-one, 14-methyl-	398	C28H46O	021857-92-1	25		



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061820\
Data File : BF120647.D
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Operator : JU/CG
Sample : L3034-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

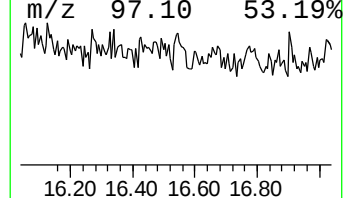
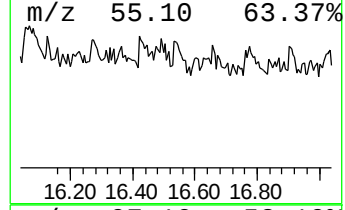
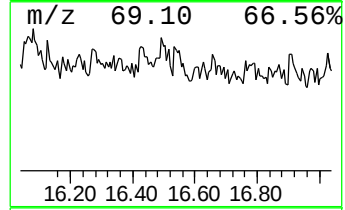
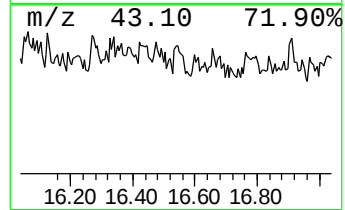
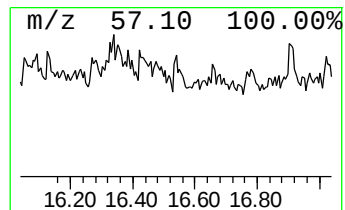
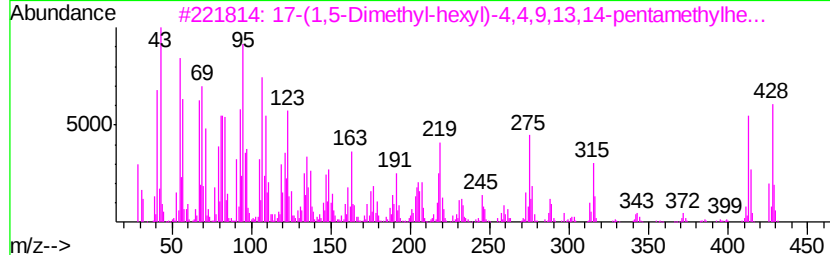
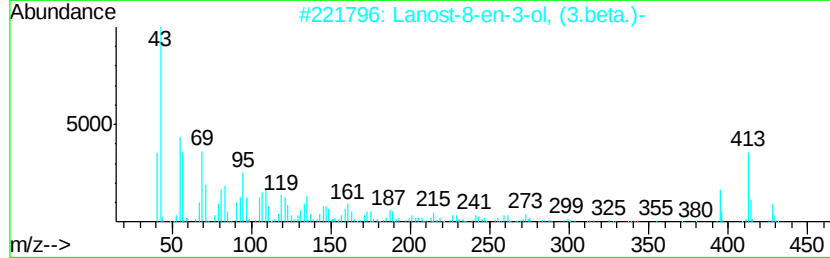
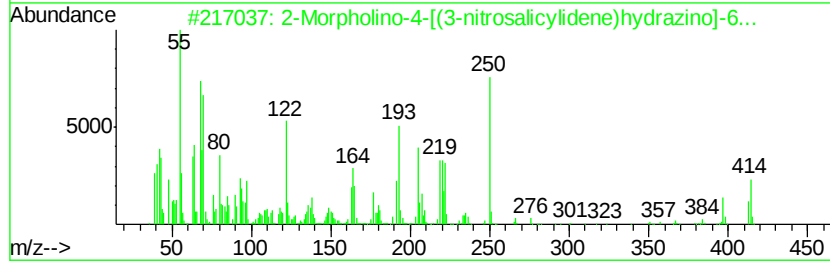
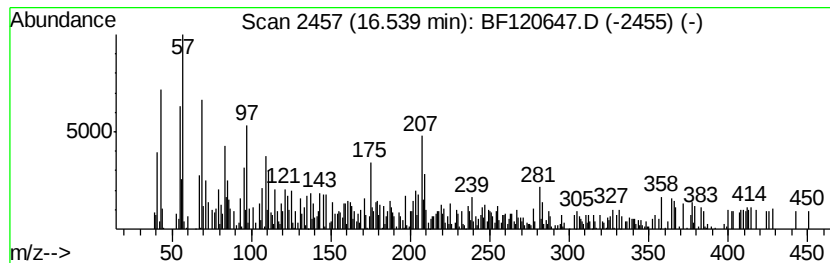
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown16.54 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.54	3.17 ng	161236	Perylene-d12		15.40	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Morpholino-4-[(3-nitrosalicyli...	414	C18H22N8O4	1000225-46-6	25	
2	Lanost-8-en-3-ol, (3.beta.)-	428	C30H52O	000079-62-9	25	
3	17-(1,5-Dimethyl-hexyl)-4,4,9,13...	428	C30H52O	1000187-63-0	11	
4	7,8-Dihydrocarpesterol	564	C37H56O4	1000214-22-4	10	
5	Cycloartanol	428	C30H52O	004657-58-3	10	



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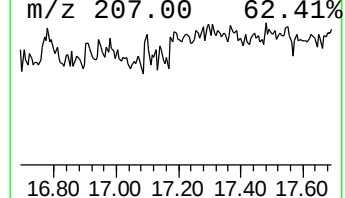
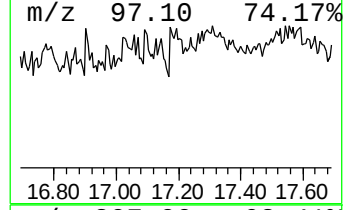
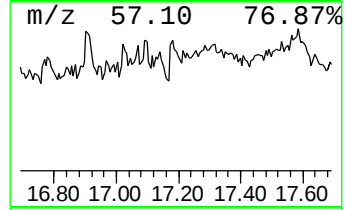
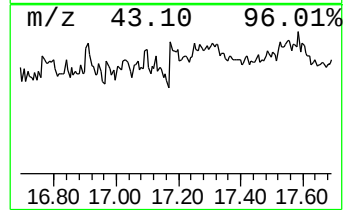
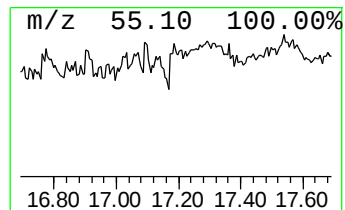
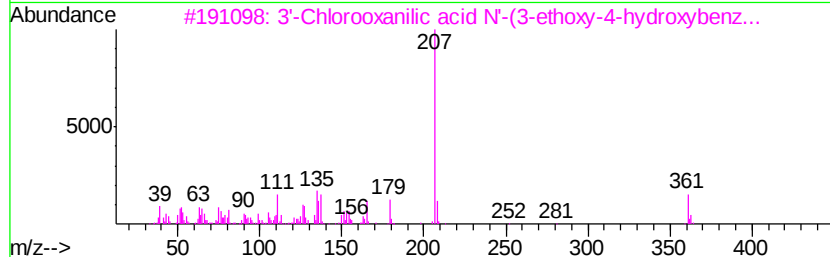
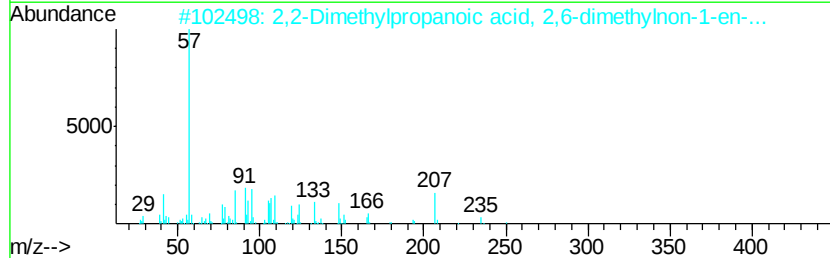
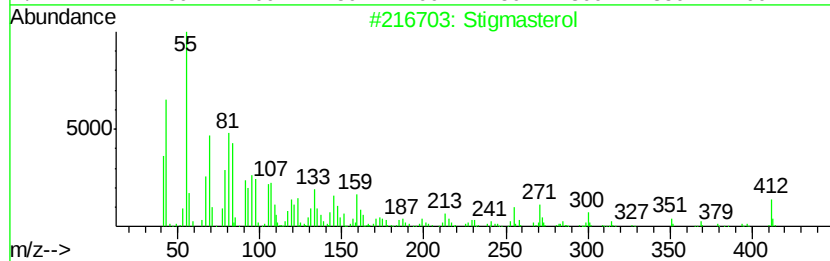
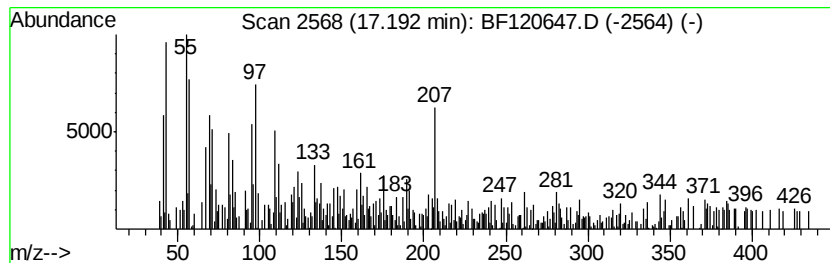
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Stigmasterol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.19	6.30 ng	320388	Perylene-d12	15.40
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Stigmasterol	412 C29H48O	000083-48-7 53
2		2,2-Dimethylpropanoic acid, 2,6-...	250 C16H26O2	1000299-33-6 51
3		3'-Chlorooxanilic acid N'-(3-eth...	361 C17H16ClN3O4	328018-74-2 45
4		4,22-Stigmastadiene-3-one	410 C29H46O	020817-72-5 43
5		3.alpha.,5-Cyclo-5.alpha.-choles...	384 C27H44O	026753-93-5 41



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061820\
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061020.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-Heneicosanol	13.80	9.4	ng	455124	5	13.96	962916	20.0
Phenanthrene, 2-d...	14.24	2.8	ng	135958	5	13.96	962916	20.0
Cyclohexanebutano...	14.40	2.2	ng	105342	5	13.96	962916	20.0
Perylene	14.97	5.4	ng	274485	6	15.40	1017630	20.0
1H-Indene, 5-buty...	15.16	6.1	ng	312098	6	15.40	1017630	20.0
unknown15.50	15.50	3.4	ng	171544	6	15.40	1017630	20.0
unknown16.05	16.05	3.4	ng	171919	6	15.40	1017630	20.0
unknown16.27	16.27	3.0	ng	152268	6	15.40	1017630	20.0
unknown16.42	16.42	2.5	ng	127416	6	15.40	1017630	20.0
unknown16.54	16.54	3.2	ng	161236	6	15.40	1017630	20.0
Stigmasterol	17.19	6.3	ng	320388	6	15.40	1017630	20.0