

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041017\
 Data File : BF094304.D
 Acq On : 10 Apr 2017 12:06
 Operator : SJ/MA
 Sample : PB98126BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB98126BL

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:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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	3.987	352	357	365	rVB	342141	399067	8.35%	1.157%
2	4.404	424	428	432	rBV	2956246	2715034	56.80%	7.871%
3	5.475	605	610	614	rBV	2402032	2731191	57.14%	7.918%
4	5.598	626	631	634	rBV	2762135	2871318	60.07%	8.324%
5	5.840	667	672	676	rBV	993248	949528	19.86%	2.753%
6	6.016	697	702	706	rBV	3064763	3265734	68.32%	9.467%
7	6.487	775	782	786	rBV	2036587	2634077	55.11%	7.636%
8	7.339	921	927	931	rBV	1232854	1279764	26.77%	3.710%
9	8.669	1145	1153	1156	rBV	3700692	4780087	100.00%	13.857%
10	9.480	1284	1291	1295	rVB	1323307	1384573	28.97%	4.014%
11	10.457	1450	1457	1461	rBV	1665705	1723381	36.05%	4.996%
12	11.304	1594	1601	1605	rBV	1371322	1383877	28.95%	4.012%
13	12.033	1719	1725	1732	rBV5	35051	76332	1.60%	0.221%
14	13.286	1930	1938	1942	rBV2	3552059	4450356	93.10%	12.901%
15	14.133	2074	2082	2093	rVB4	57422	176036	3.68%	0.510%
16	14.551	2148	2153	2158	rBV	1146235	1273013	26.63%	3.690%
17	15.033	2226	2235	2246	rBV5	145874	438883	9.18%	1.272%
18	15.715	2345	2351	2358	rBV2	92282	195333	4.09%	0.566%
19	16.180	2425	2430	2439	rVB	795620	912973	19.10%	2.647%
20	16.309	2446	2452	2458	rVB2	83102	165087	3.45%	0.479%
21	16.615	2498	2504	2512	rBV8	73794	193290	4.04%	0.560%
22	16.962	2557	2563	2573	rVB4	58908	158118	3.31%	0.458%
23	17.080	2580	2583	2587	rVB5	43023	70258	1.47%	0.204%
24	19.368	2967	2972	2985	rVB5	84444	267719	5.60%	0.776%

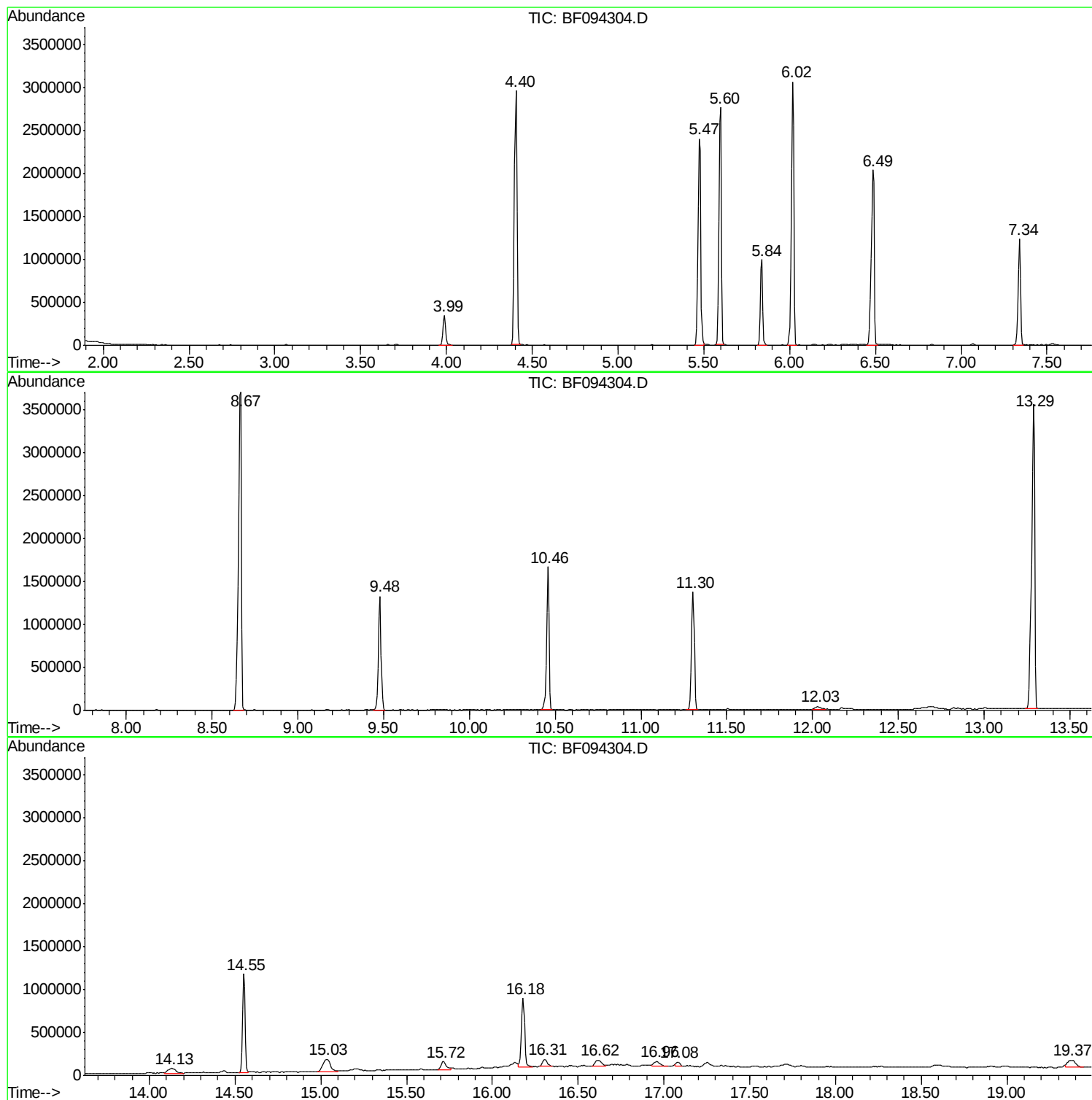
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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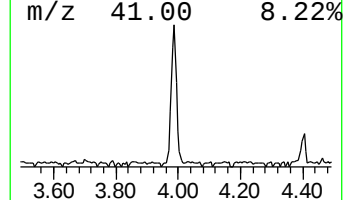
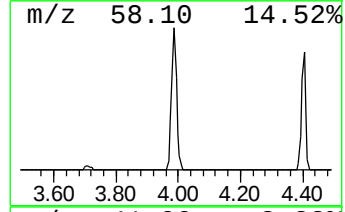
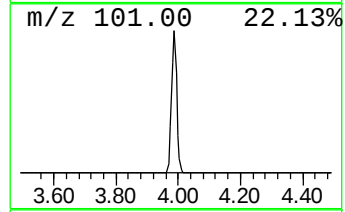
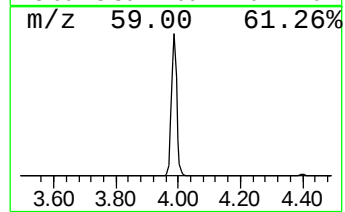
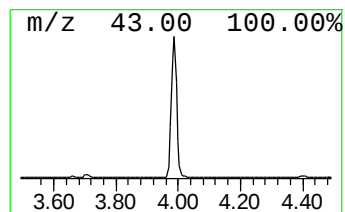
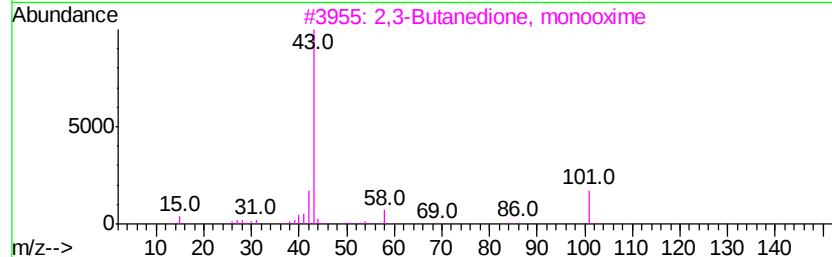
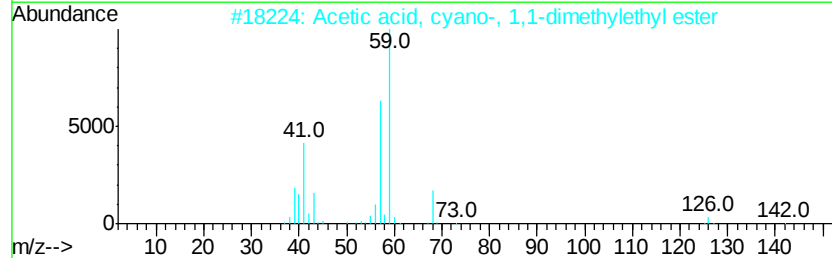
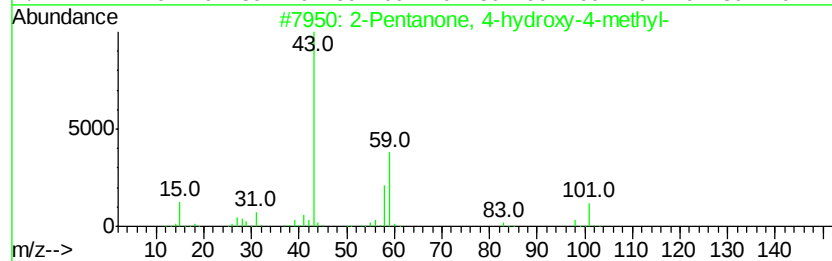
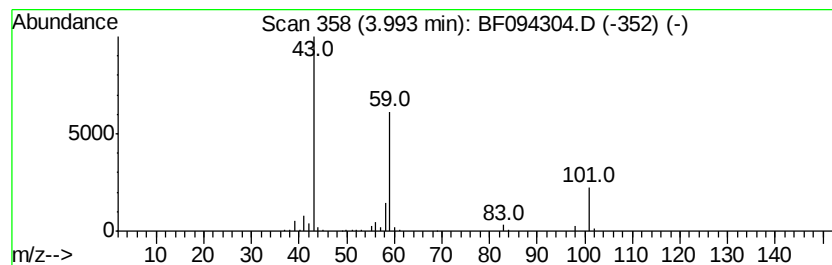
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.99	8.41 ng	399067	1,4-Dichlorobenzene-d4	5.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9



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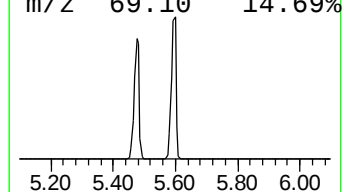
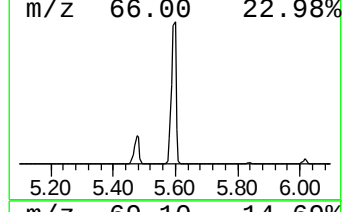
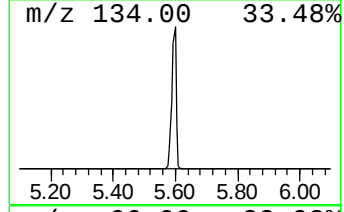
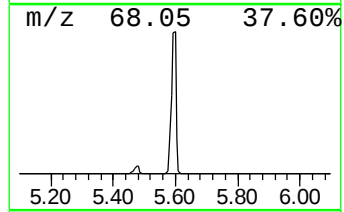
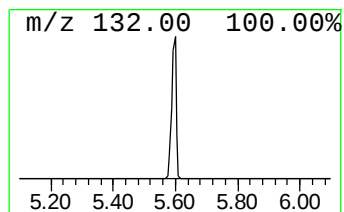
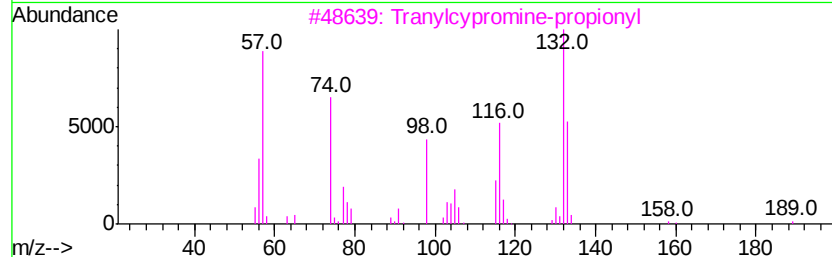
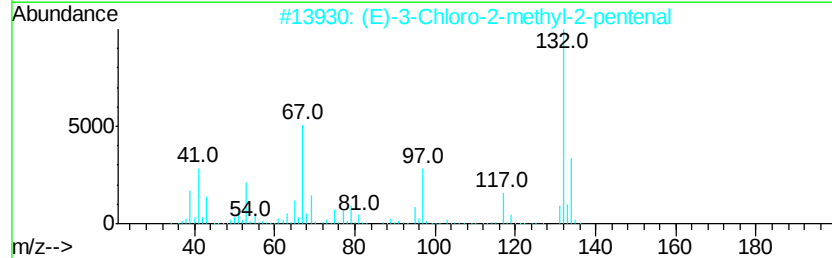
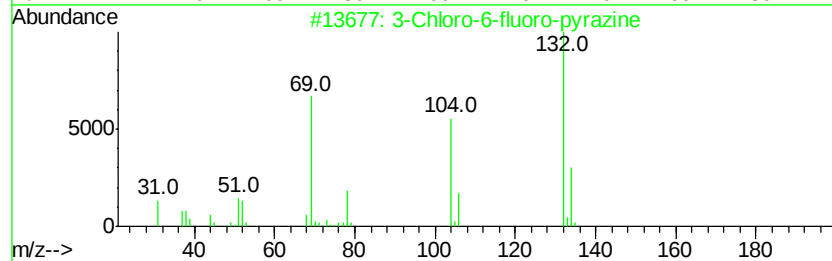
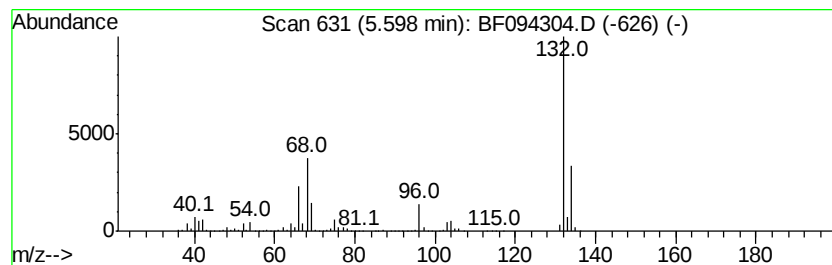
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown5.60 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.60	60.48 ng	2871320	1,4-Dichlorobenzene-d4	5.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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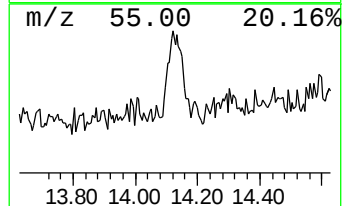
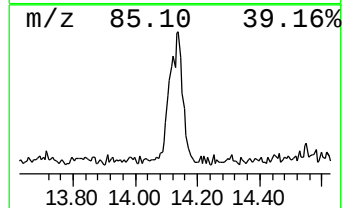
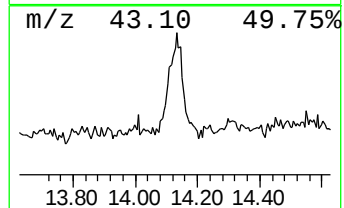
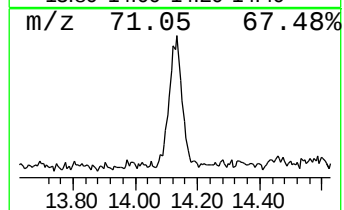
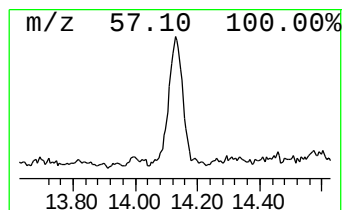
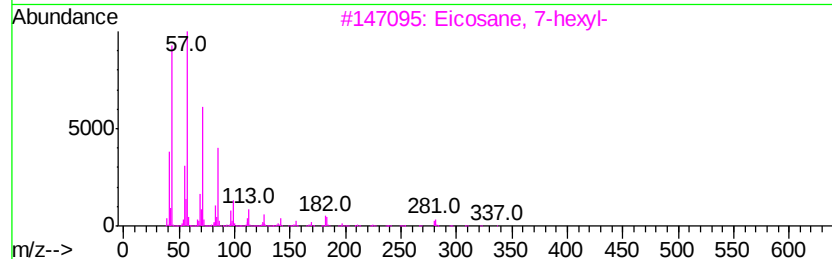
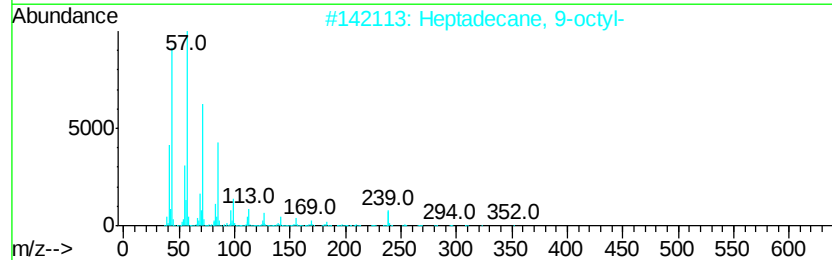
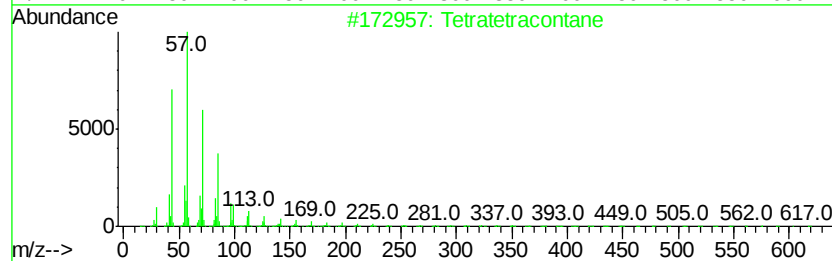
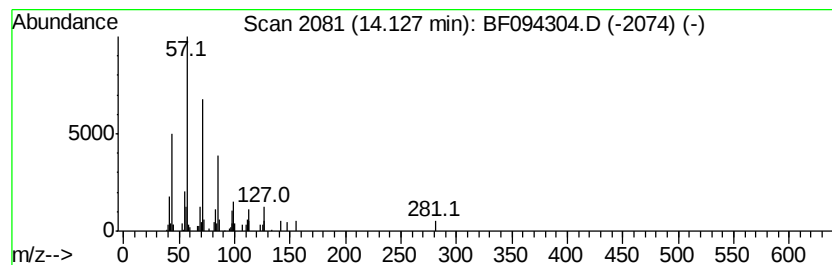
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Peak Number 4 Tetratetracontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.13	2.77 ng	176036	Chrysene-d12	14.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratetracontane	619	C44H90	007098-22-8	91
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
3		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
4		Nonacosane	408	C29H60	000630-03-5	90
5		Octacosane	394	C28H58	000630-02-4	87



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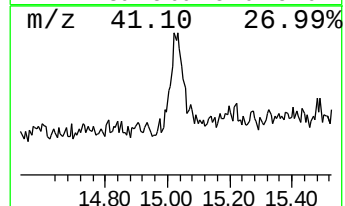
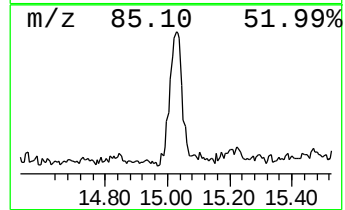
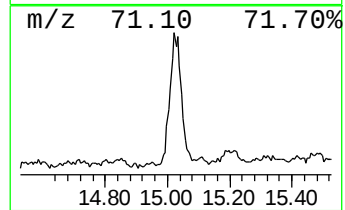
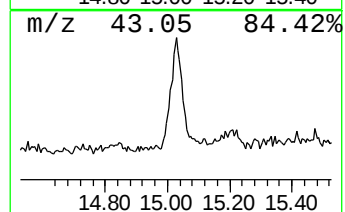
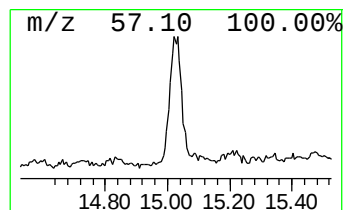
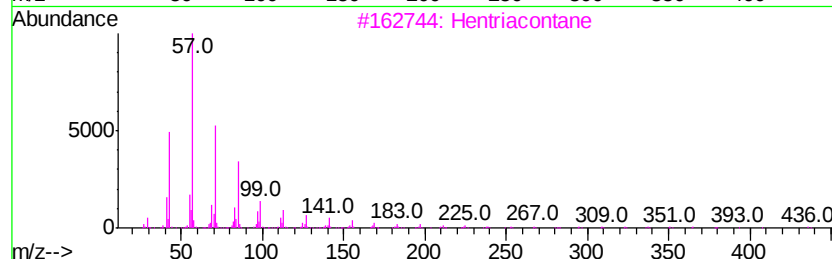
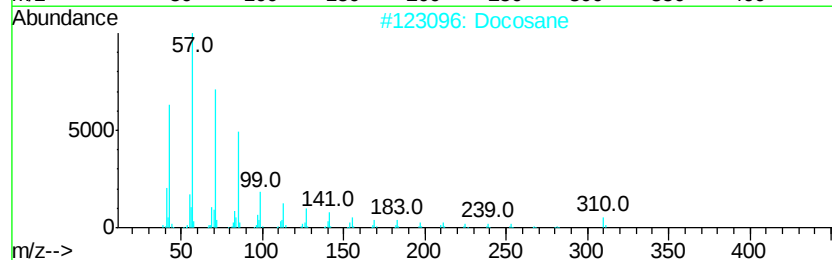
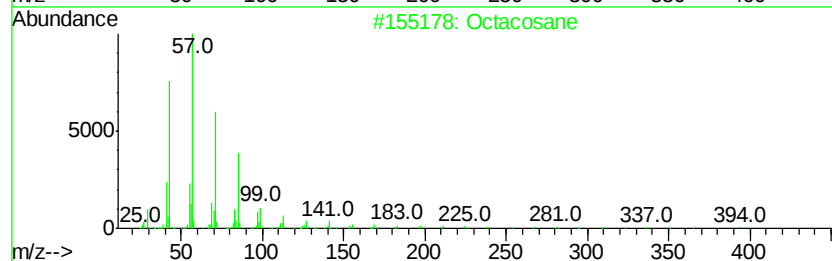
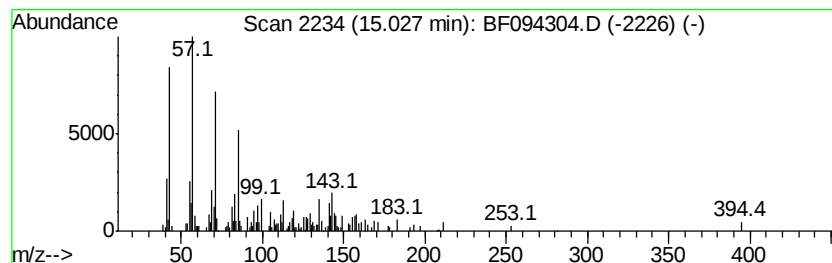
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.03	6.90 ng	438883	Chrysene-d12	14.55

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	53
2	Docosane		310	C22H46	000629-97-0	49
3	Hentriacontane		437	C31H64	000630-04-6	49
4	Heneicosane		296	C21H44	000629-94-7	46
5	Tetratriacontane		479	C34H70	014167-59-0	46



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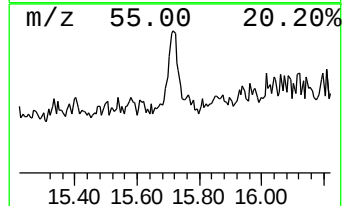
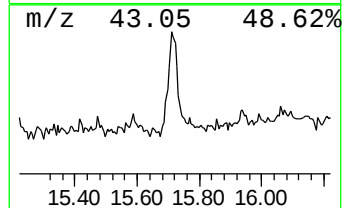
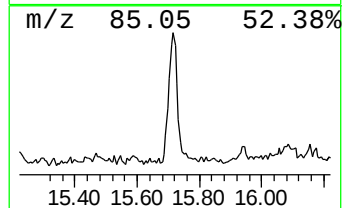
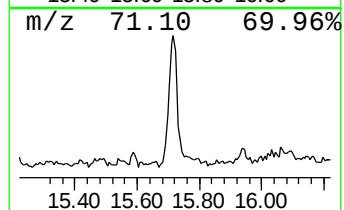
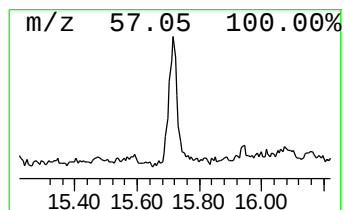
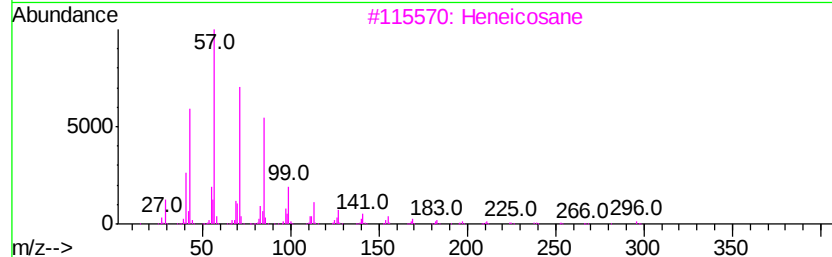
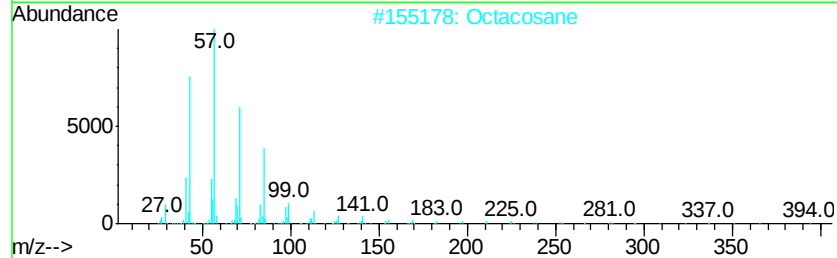
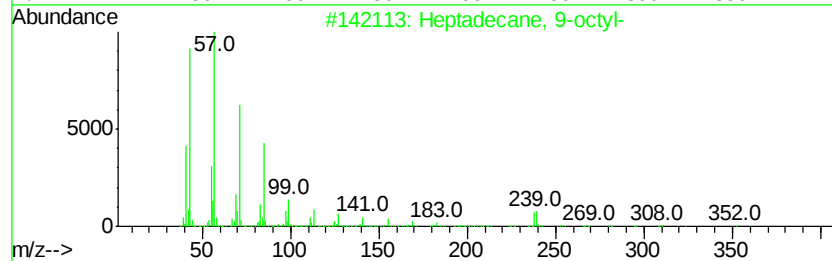
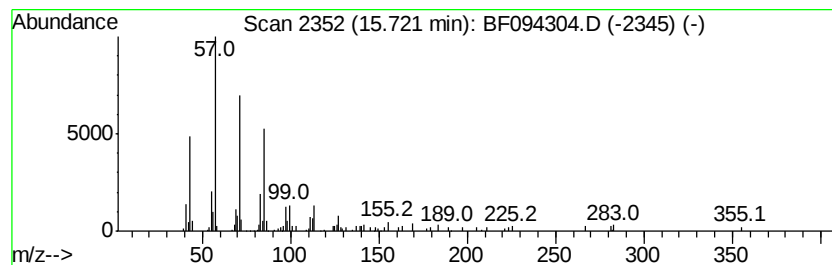
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Peak Number 6 Heptadecane, 9-octyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.72	4.28 ng	195333	Perylene-d12	16.18	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	90
5	Eicosane	282	C20H42	000112-95-8	90



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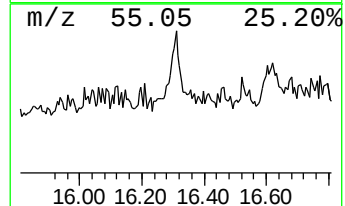
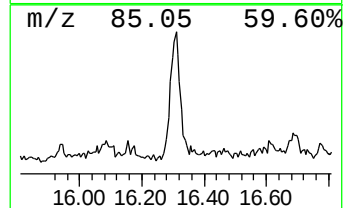
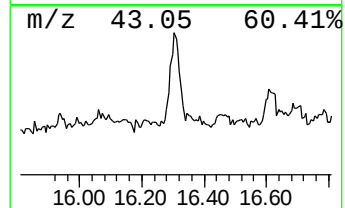
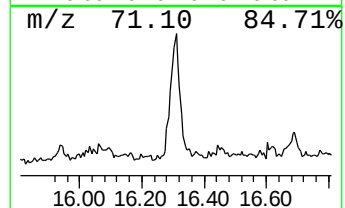
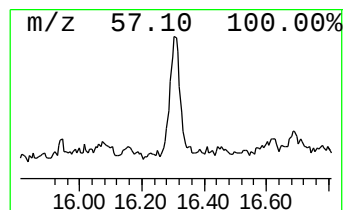
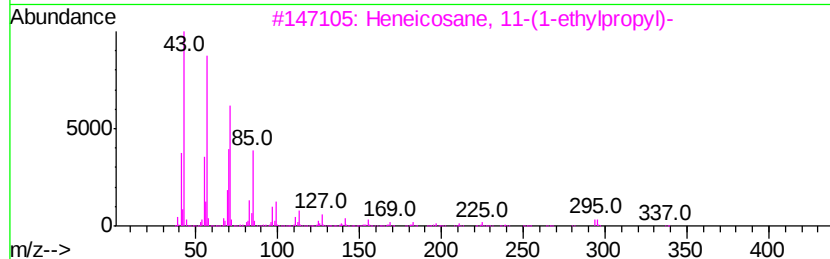
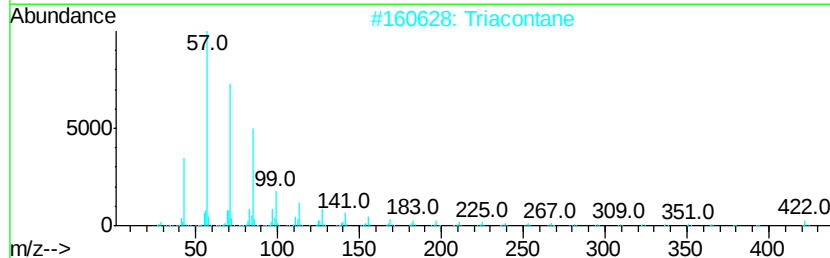
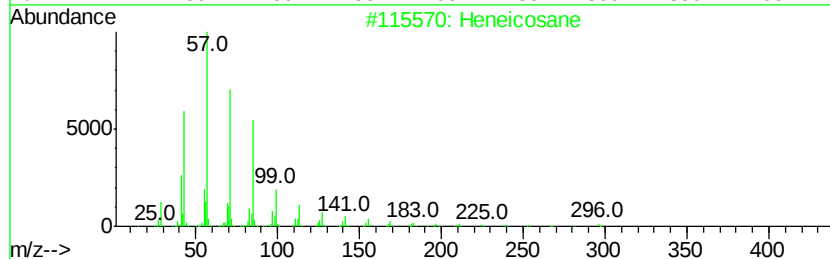
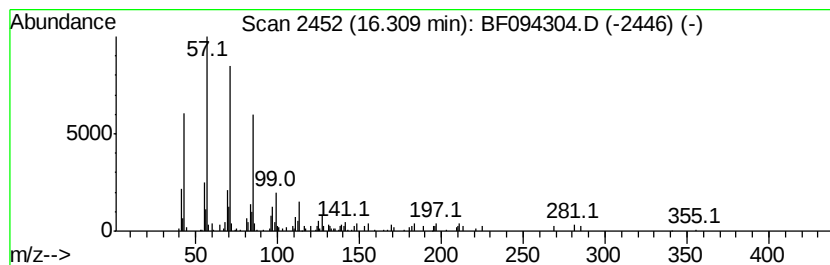
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.31	3.62 ng	165087	Perylene-d12	16.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Triacontane	422	C30H62	000638-68-6	90
3		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
4		Tetracosane	338	C24H50	000646-31-1	87
5		Hexadecane	226	C16H34	000544-76-3	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF041017\
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Acq On : 10 Apr 2017 12:06
Operator : SJ/MA
Sample : PB98126BL
Misc :
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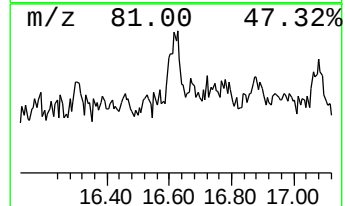
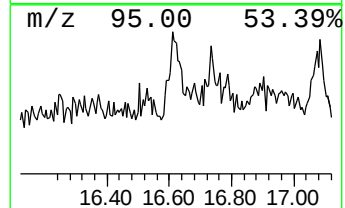
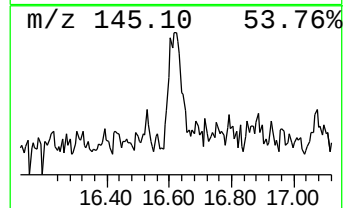
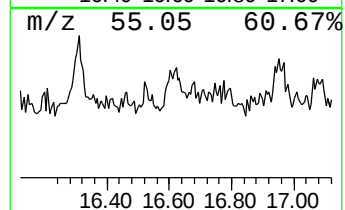
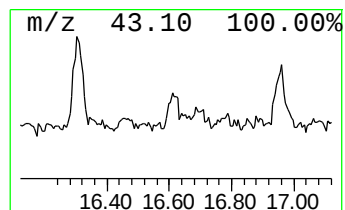
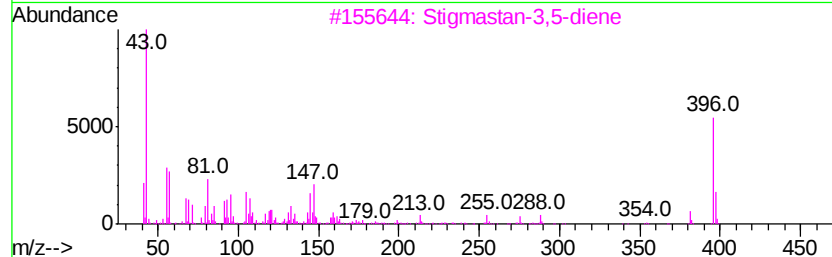
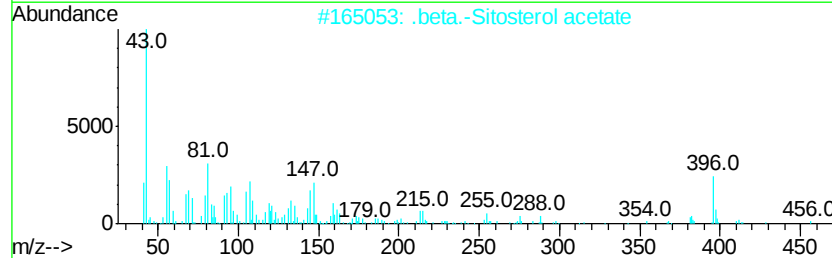
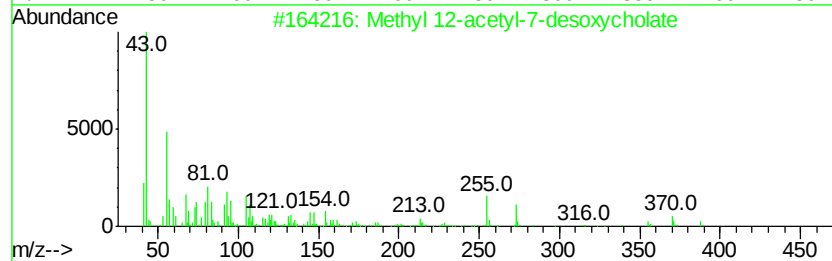
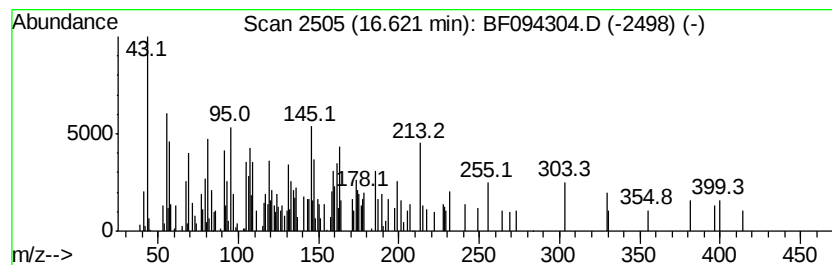
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown16.62 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.62	4.23 ng	193290	Perylene-d12	16.18	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 12-acetyl-7-desoxycholate	448	C27H44O5	055547-48-3	37
2	.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	32
3	Stigmastan-3,5-diene	396	C29H48	1000214-16-4	10
4	Norflurazon	303	C12H9ClF3N3O	027314-13-2	9
5	2,6-Dichloronitrosobenzene	175	C6H3Cl2NO	001194-66-7	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF041017\
Data File : BF094304.D
Acq On : 10 Apr 2017 12:06
Operator : SJ/MA
Sample : PB98126BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB98126BL

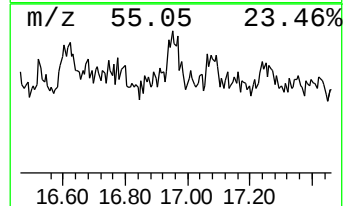
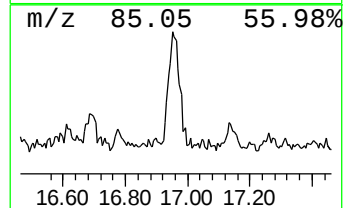
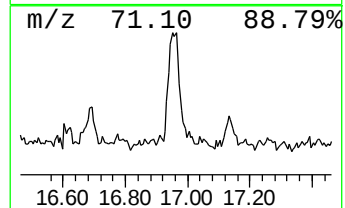
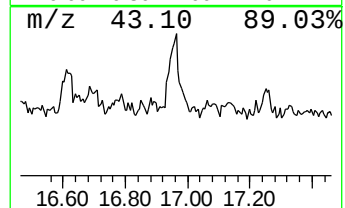
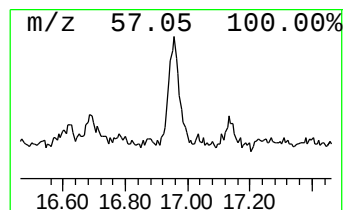
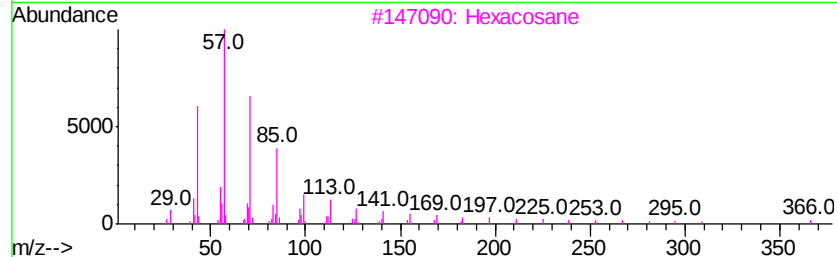
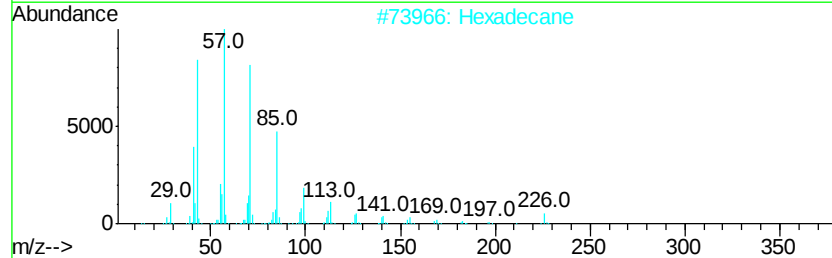
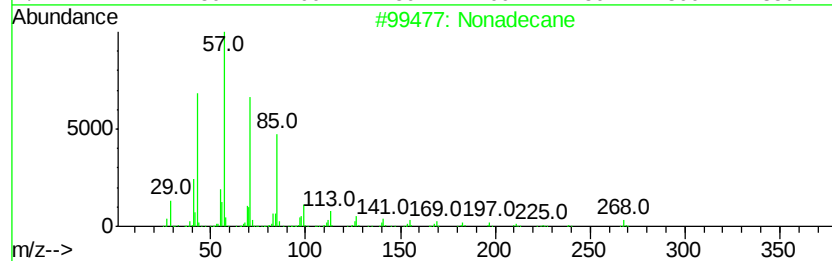
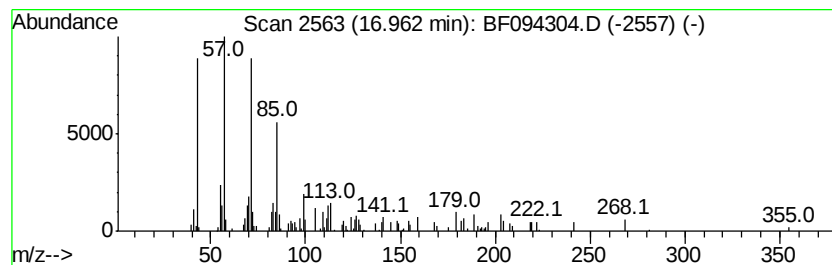
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.96	3.46 ng	158118	Perylene-d12	16.18

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	76
2	Hexadecane		226	C16H34	000544-76-3	64
3	Hexacosane		366	C26H54	000630-01-3	64
4	Heneicosane		296	C21H44	000629-94-7	64
5	Eicosane		282	C20H42	000112-95-8	59



Data Path : Z:\HPCHEM1\BNA F\DATA\BF041017\
Data File : BF094304.D
Acq On : 10 Apr 2017 12:06
Operator : SJ/MA
Sample : PB98126BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
PB98126BL

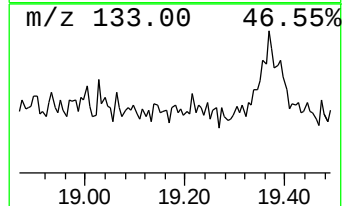
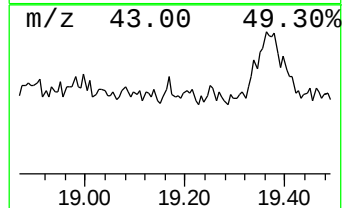
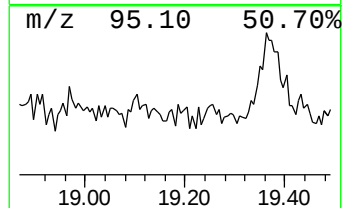
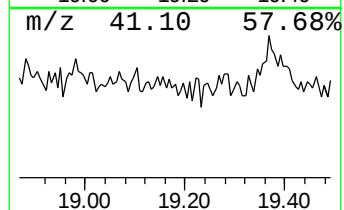
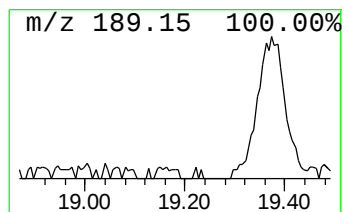
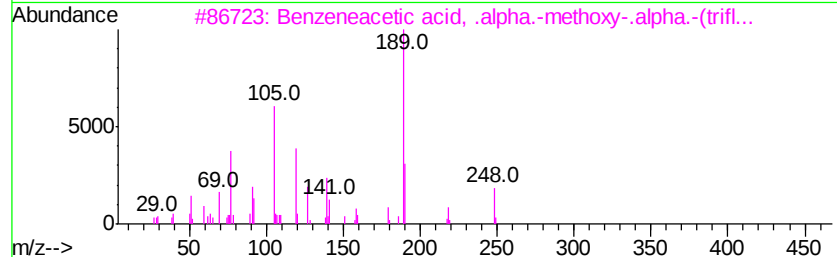
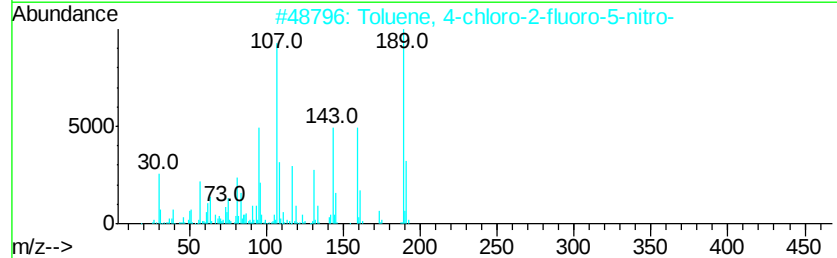
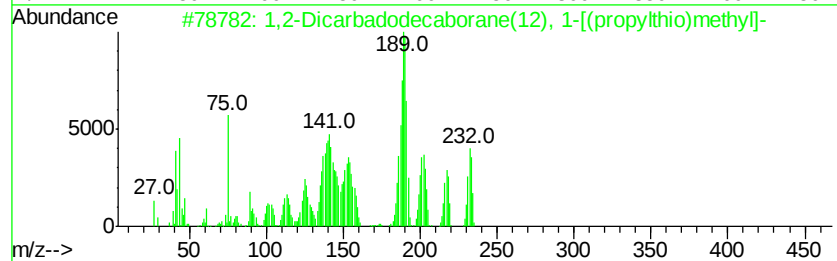
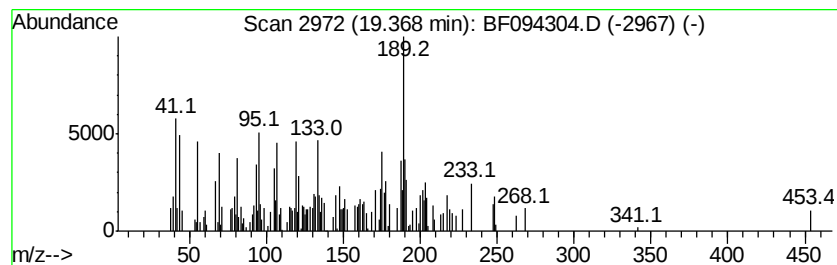
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown19.37 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.37	5.86 ng	267719	Perylene-d12	16.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Dicarbododecaborane(12), 1-[...	234	C6H20B10S	062906-36-9	38
2		Toluene, 4-chloro-2-fluoro-5-nitro-	189	C7H5ClFN02	018349-11-6	27
3		Benzeneacetic acid, .alpha.-meth...	248	C11H11F303	077611-72-4	25
4		6-Bromo-9-phenanthrene diazometh...	324	C16H9BrN20	1000254-49-2	22
5		Ethanone, 1-[4-(trifluoromethoxy...	204	C9H7F302	085013-98-5	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041017\
Data File : BF094304.D
Acq On : 10 Apr 2017 12:06
Operator : SJ/MA
Sample : PB98126BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB98126BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	3.99	8.4	ng	399067	1	5.84	949528	20.0
unknown5.60	5.60	60.5	ng	2871320	1	5.84	949528	20.0
Tetratetracontane	14.13	2.8	ng	176036	5	14.55	1273010	20.0
Octacosane	15.03	6.9	ng	438883	5	14.55	1273010	20.0
Heptadecane, 9-oc...	15.72	4.3	ng	195333	6	16.18	912973	20.0
Heneicosane	16.31	3.6	ng	165087	6	16.18	912973	20.0
unknown16.62	16.62	4.2	ng	193290	6	16.18	912973	20.0
Nonadecane	16.96	3.5	ng	158118	6	16.18	912973	20.0
unknown19.37	19.37	5.9	ng	267719	6	16.18	912973	20.0