

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042816\
 Data File : BF086476.D
 Acq On : 28 Apr 2016 21:25
 Operator : UM/SJ
 Sample : H2654-05
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 26WARD-2A-CS-14(6-12FTBGS)

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:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.967	250	252	260	rVB	66019	116936	2.57%	0.307%
2	5.379	285	288	291	rBV	3092627	3592302	79.01%	9.426%
3	6.430	376	380	382	rBV	3294074	4546544	100.00%	11.930%
4	6.556	388	391	393	rBV	3941039	4187656	92.11%	10.988%
5	6.625	393	397	399	rVB	29905	50462	1.11%	0.132%
6	6.785	409	411	416	rBV	1143370	1058932	23.29%	2.779%
7	6.945	422	425	427	rBV	3048708	3059208	67.29%	8.027%
8	7.356	458	461	463	rBV	2388073	2802165	61.63%	7.353%
9	7.447	467	469	477	rVB	55289	120710	2.65%	0.317%
10	8.076	521	524	526	rBV	1097557	1315425	28.93%	3.452%
11	9.150	615	618	621	rBV	3739370	3775202	83.03%	9.906%
12	9.550	651	653	655	rBV	287675	384643	8.46%	1.009%
13	9.768	663	672	674	rBV	106256	120057	2.64%	0.315%
14	9.825	674	677	679	rBV	1690266	1483761	32.63%	3.893%
15	10.259	712	715	717	rBV2	122767	177660	3.91%	0.466%
16	10.488	731	735	738	rBV	57572	108009	2.38%	0.283%
17	10.613	743	746	748	rBV	2447210	2494500	54.87%	6.546%
18	10.739	755	757	763	rVB	182391	257939	5.67%	0.677%
19	10.934	772	774	776	rBV2	25321	47252	1.04%	0.124%
20	11.185	792	796	797	rBV	121333	112990	2.49%	0.296%
21	11.311	804	807	809	rBV	902036	1268284	27.90%	3.328%
22	11.608	831	833	838	rVB	50318	48553	1.07%	0.127%
23	12.511	909	912	918	rBV	102486	113699	2.50%	0.298%
24	12.739	928	932	934	rBV	93651	135818	2.99%	0.356%
25	12.888	943	945	948	rBV	2420734	3036406	66.78%	7.968%
26	13.128	962	966	968	rBV	45060	54220	1.19%	0.142%
27	13.471	993	996	999	rBV	50498	59021	1.30%	0.155%
28	13.791	1021	1024	1030	rBV	298944	414776	9.12%	1.088%
29	13.940	1034	1037	1045	rVV	568414	1001519	22.03%	2.628%
30	14.420	1077	1079	1081	rBV2	32520	48956	1.08%	0.128%
31	14.694	1101	1103	1108	rBV4	23473	56539	1.24%	0.148%
32	14.945	1123	1125	1129	rBV	32111	70192	1.54%	0.184%
33	15.334	1156	1159	1167	rVV	593547	890974	19.60%	2.338%
34	15.780	1196	1198	1200	rBV	35898	46087	1.01%	0.121%

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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:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.825	1200	1202	1210	rVB5	25968	66850	1.47%	0.175%
36	16.248	1236	1239	1244	rBV2	43052	94295	2.07%	0.247%
37	16.728	1277	1281	1284	rBV	350054	651970	14.34%	1.711%
38	16.785	1284	1286	1289	rVB	38049	70746	1.56%	0.186%
39	18.008	1389	1393	1401	rVB3	56981	168605	3.71%	0.442%

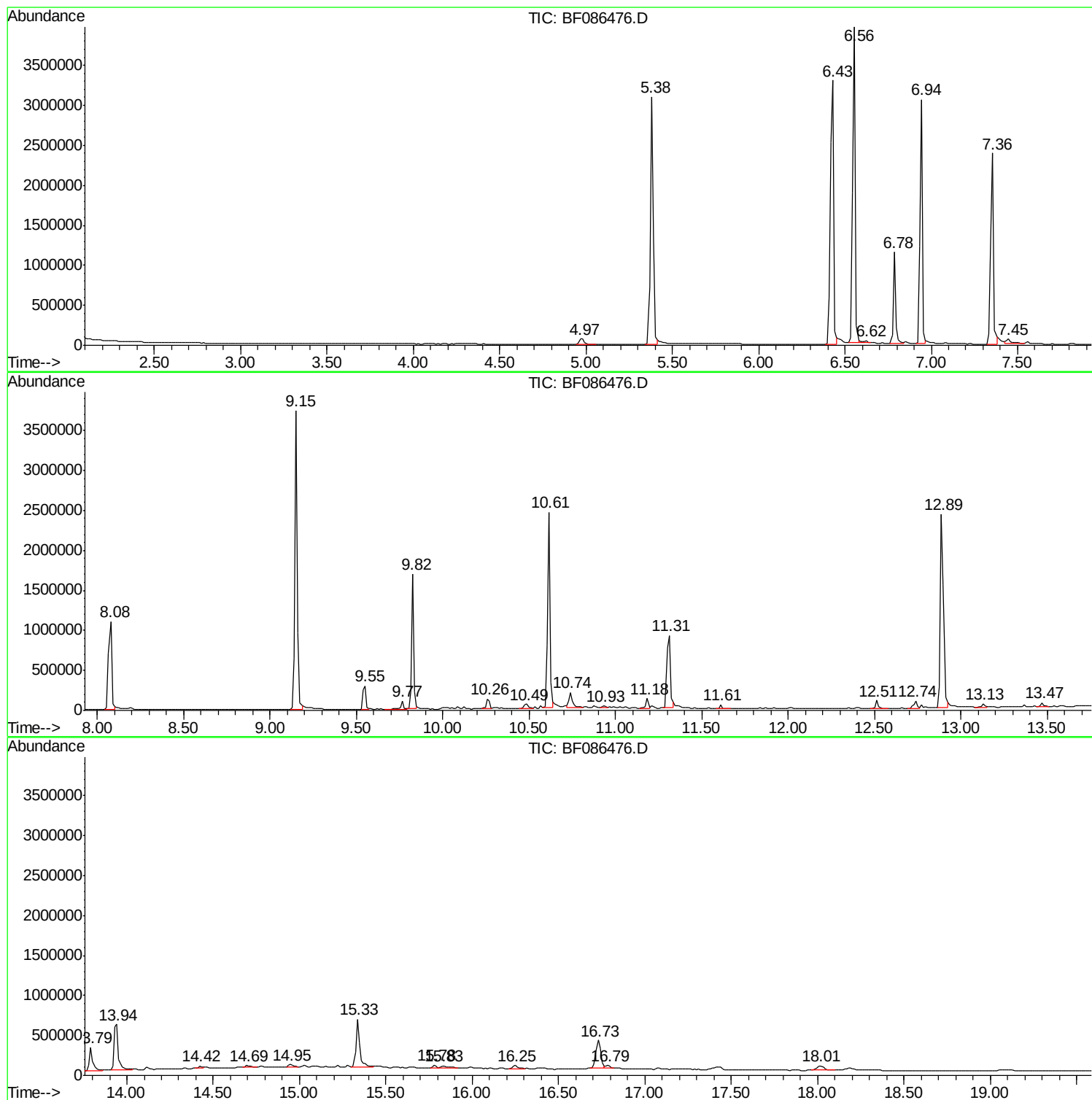
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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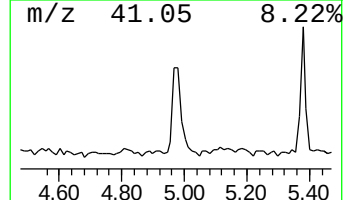
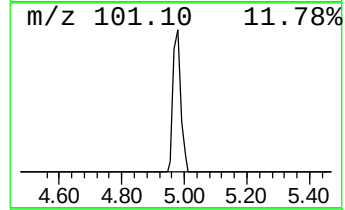
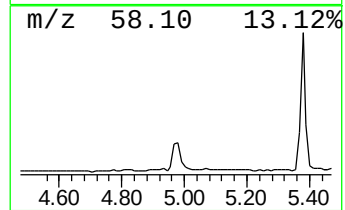
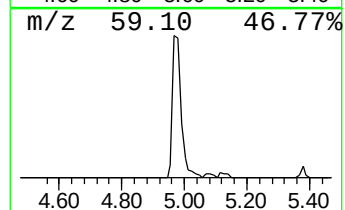
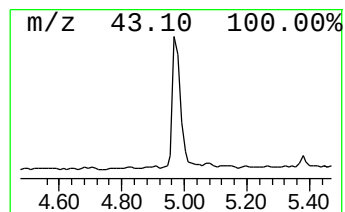
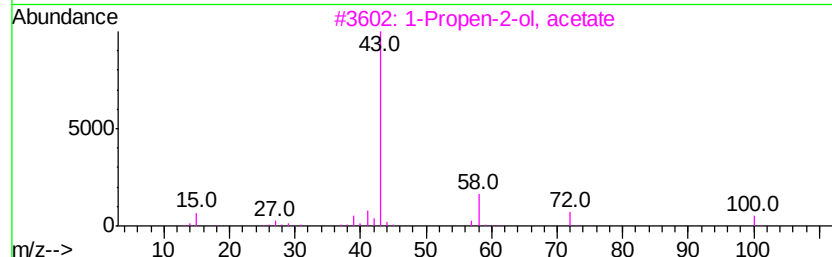
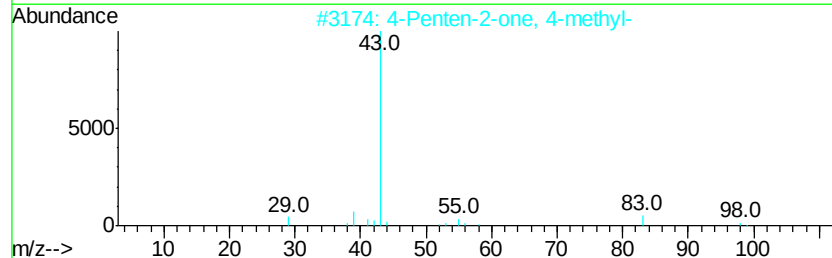
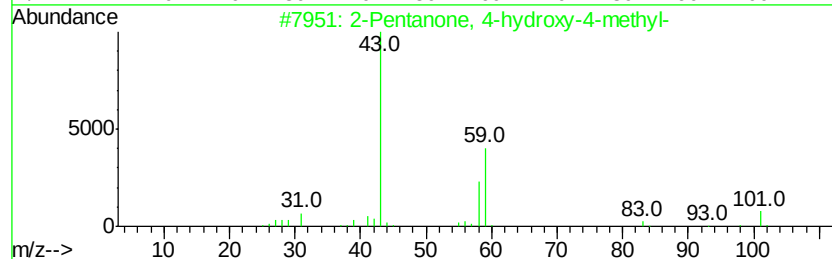
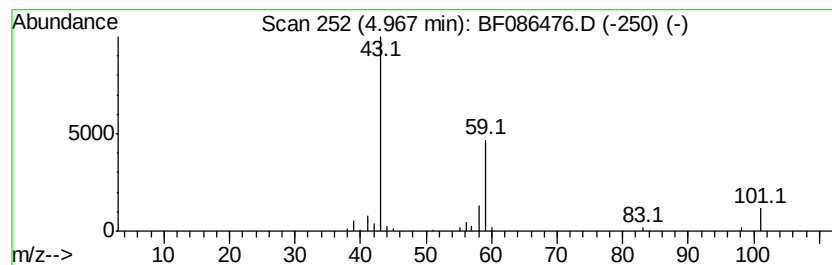
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	2.21 ng	116936	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	10
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
4		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5		dl-4-Amino-3-hydroxybutyric acid	119	C4H9NO3	000352-21-6	9



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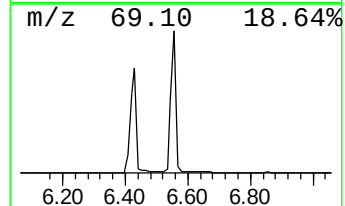
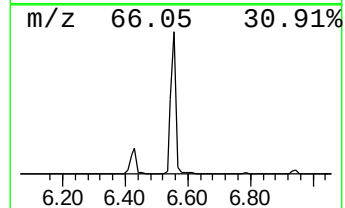
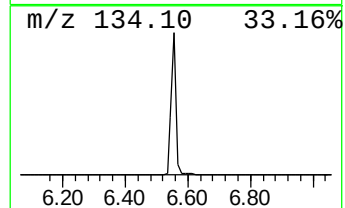
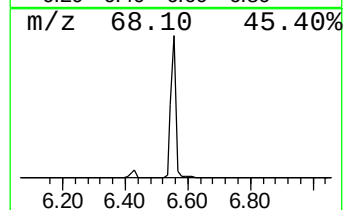
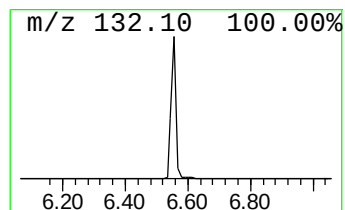
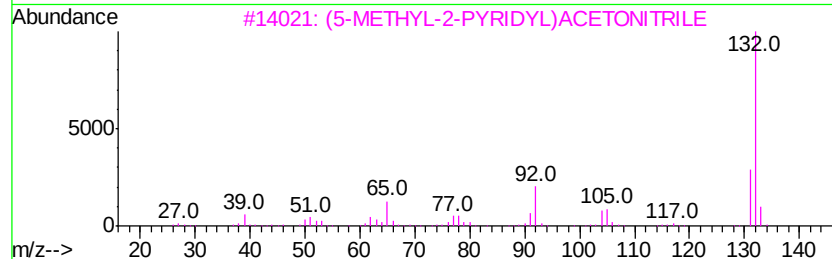
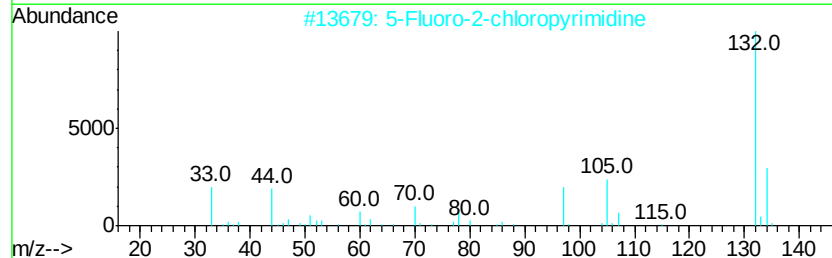
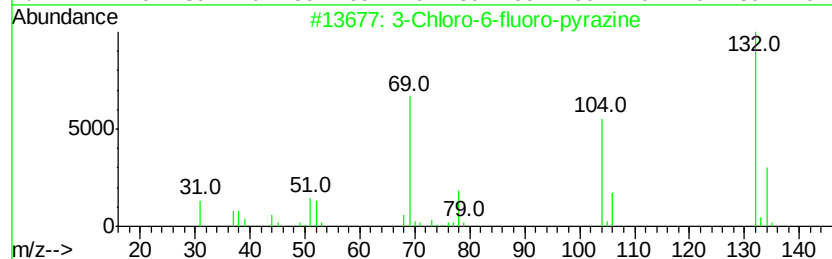
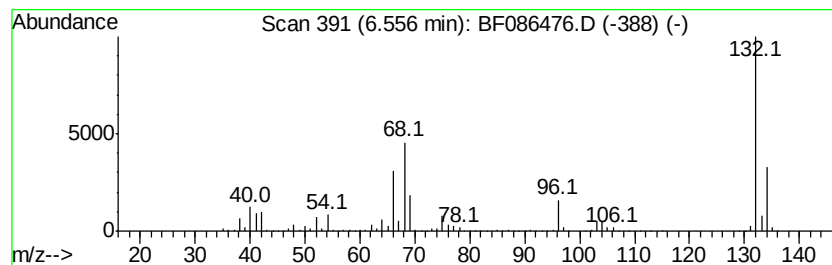
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	79.09 ng	4187660	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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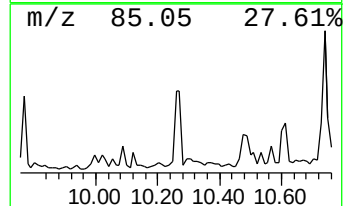
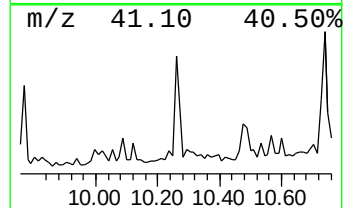
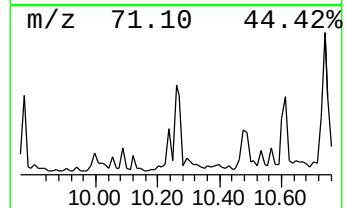
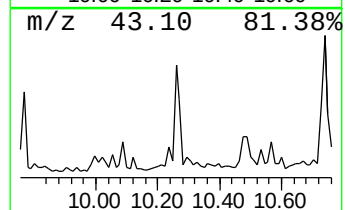
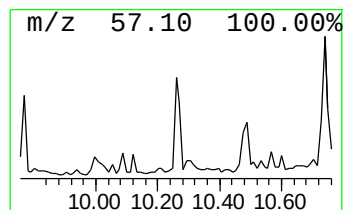
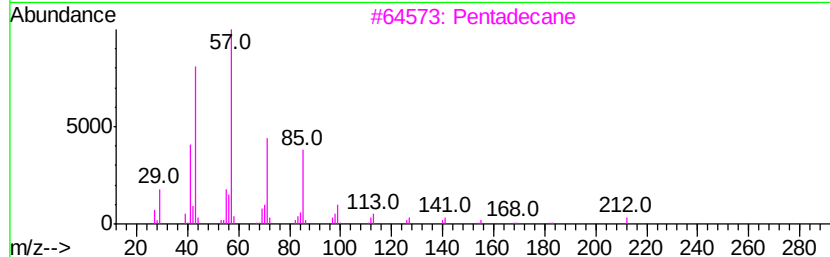
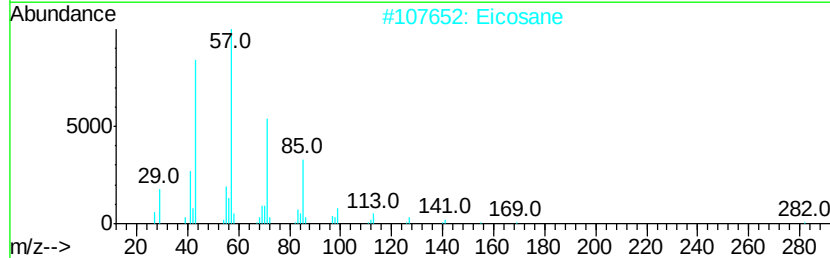
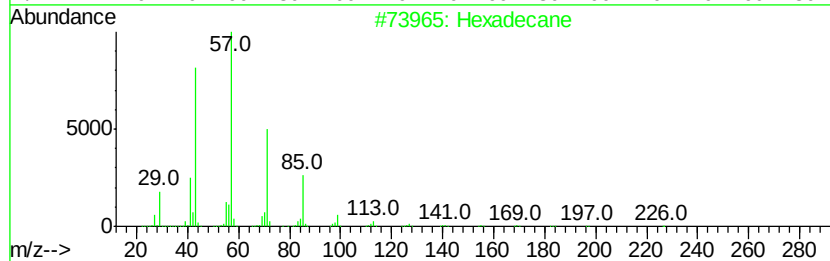
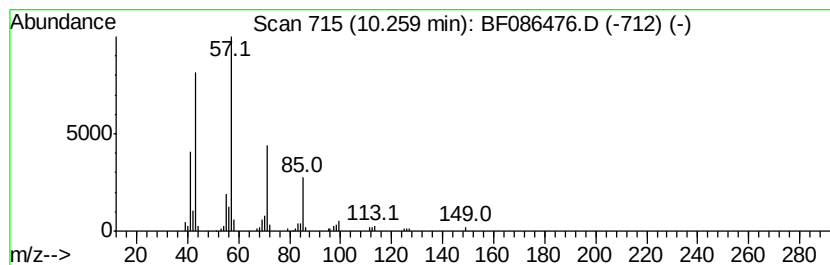
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.26	2.39 ng	177660	Acenaphthene-d10	9.82
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	91
2	Eicosane	282 C20H42	000112-95-8	91
3	Pentadecane	212 C15H32	000629-62-9	80
4	Octadecane	254 C18H38	000593-45-3	72
5	Tridecane	184 C13H28	000629-50-5	72



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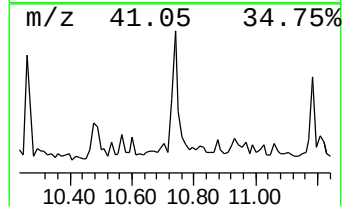
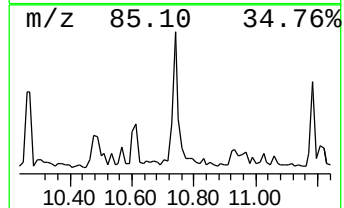
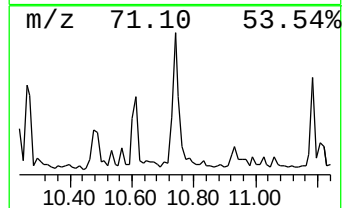
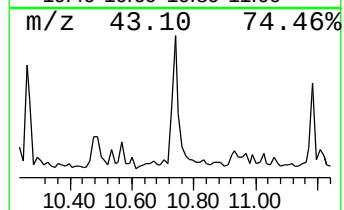
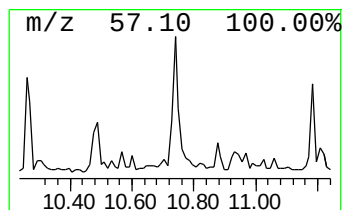
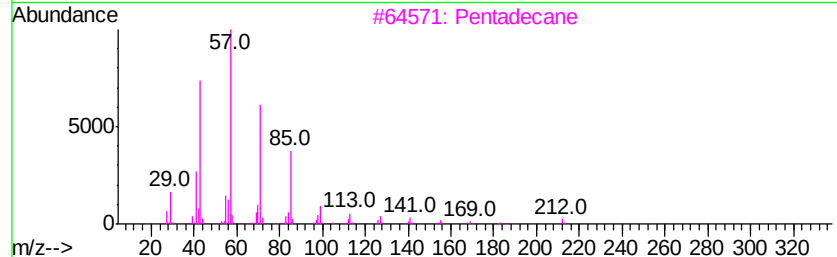
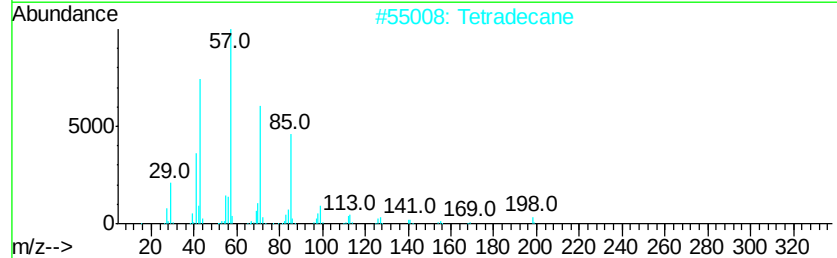
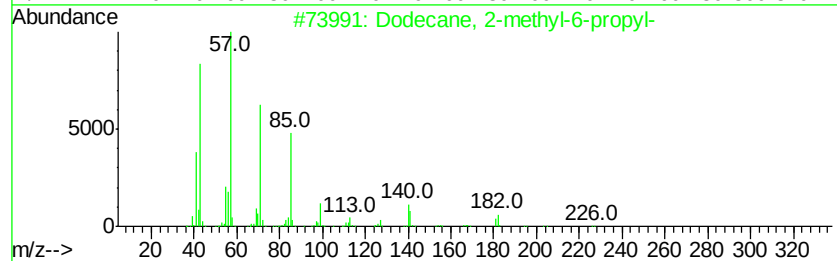
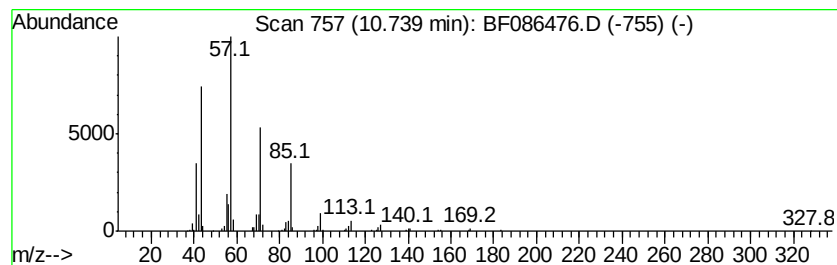
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Dodecane, 2-methyl-6-propyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	4.07 ng	257939	Phenanthrene-d10	11.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	90
2		Tetradecane	198	C14H30	000629-59-4	90
3		Pentadecane	212	C15H32	000629-62-9	90
4		Hexadecane	226	C16H34	000544-76-3	90
5		Eicosane	282	C20H42	000112-95-8	90



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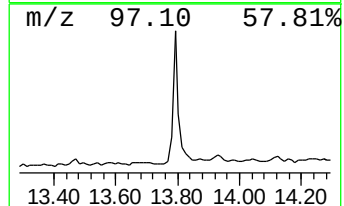
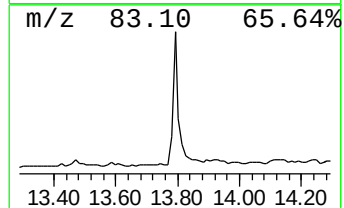
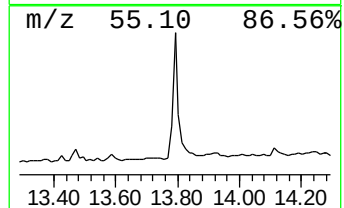
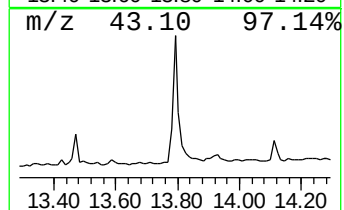
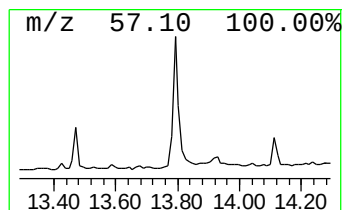
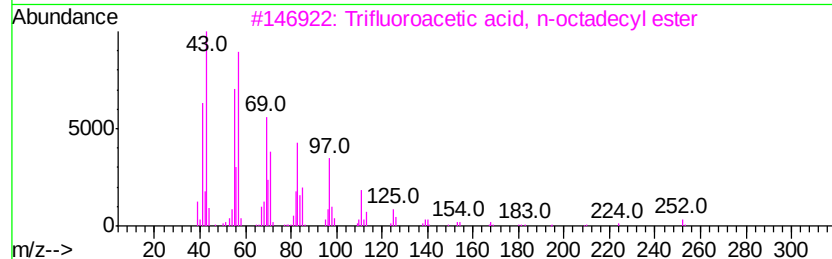
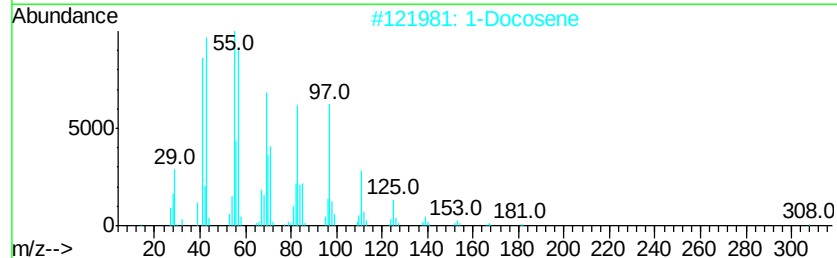
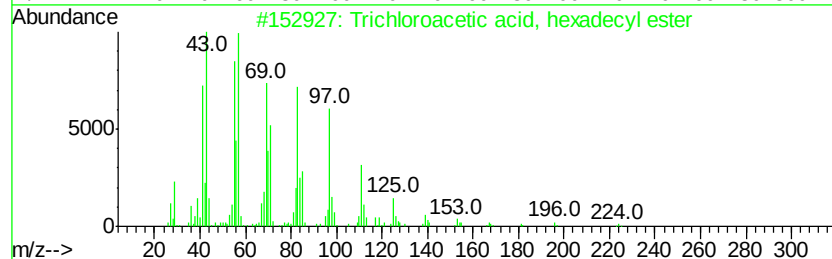
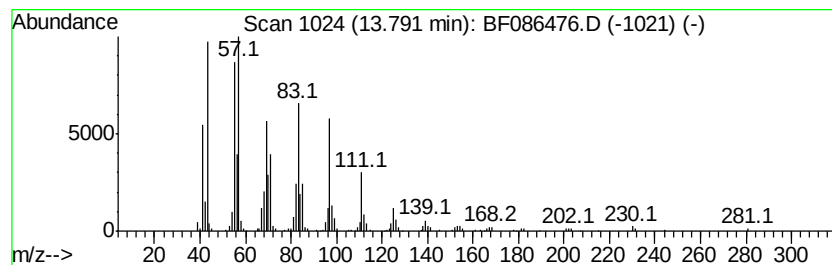
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	8.28 ng	414776	Chrysene-d12	13.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2		1-Docosene	308	C22H44	001599-67-3	95
3		Trifluoroacetic acid, n-octadecyl...	366	C20H37F3O2	079392-43-1	91
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5		11-Tricosene	322	C23H46	052078-56-5	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042816\
Data File : BF086476.D
Acq On : 28 Apr 2016 21:25
Operator : UM/SJ
Sample : H2654-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
26WARD-2A-CS-14(6-12FTBGS)

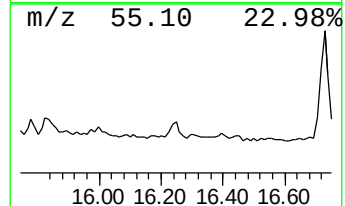
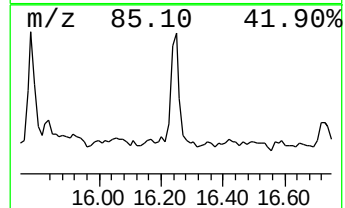
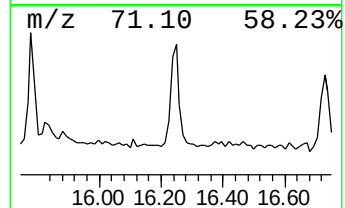
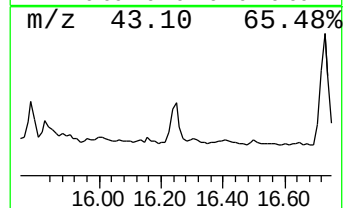
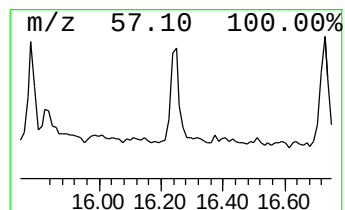
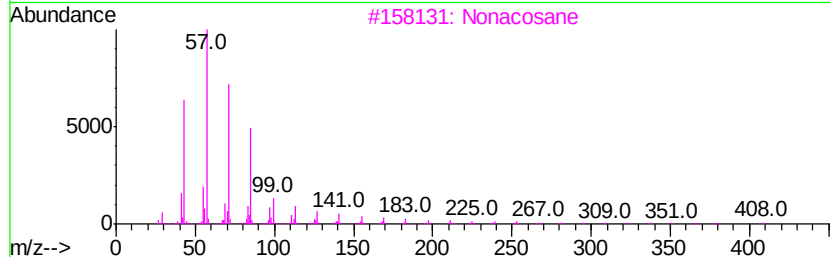
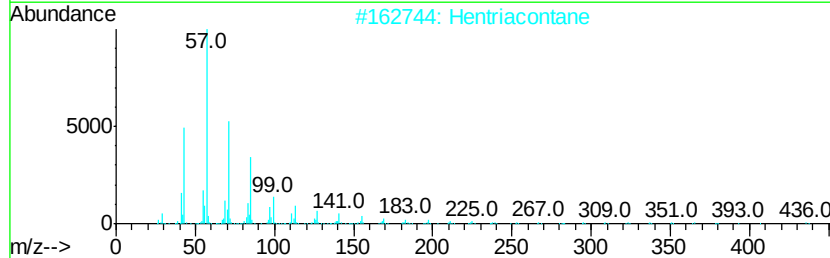
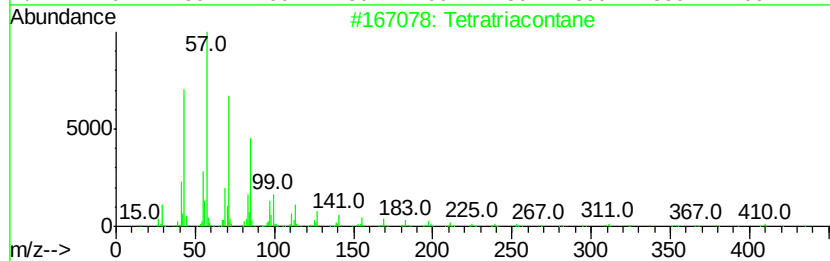
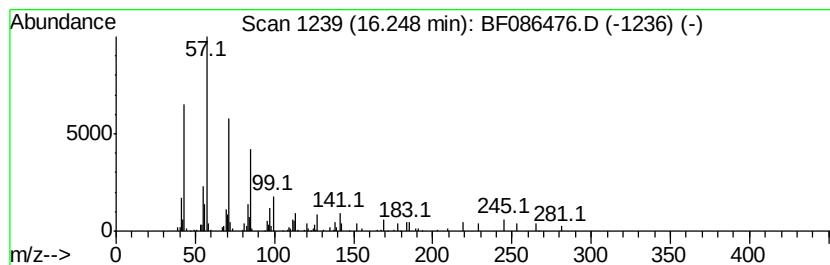
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetratriacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.25	2.12 ng	94295	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratriacontane	479	C34H70	014167-59-0	87
2	Hentriacontane	437	C31H64	000630-04-6	87
3	Nonacosane	408	C29H60	000630-03-5	86
4	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	86
5	Nonadecane, 2,3-dimethyl-	296	C21H44	075163-99-4	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042816\
Data File : BF086476.D
Acq On : 28 Apr 2016 21:25
Operator : UM/SJ
Sample : H2654-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
26WARD-2A-CS-14(6-12FTBGS)

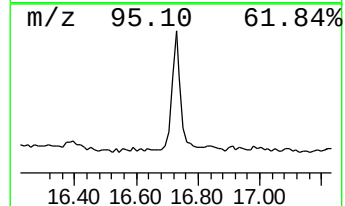
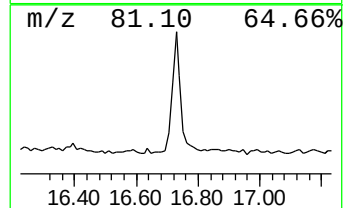
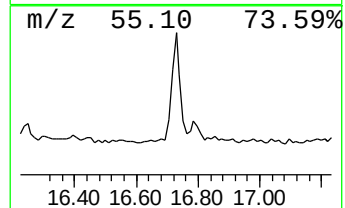
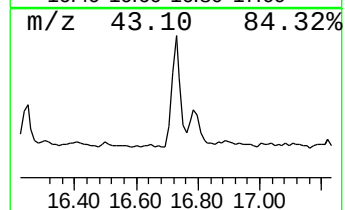
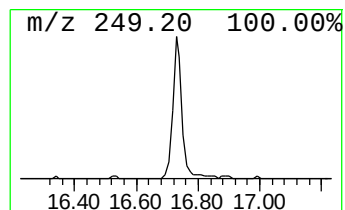
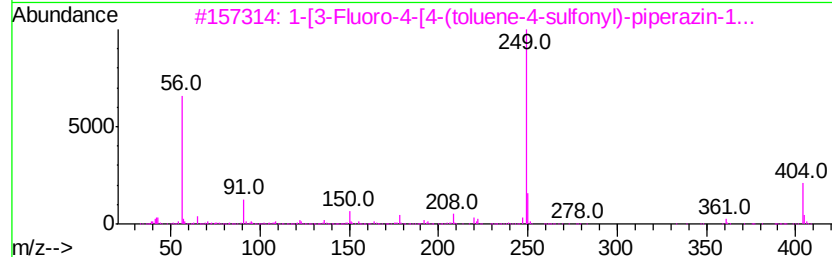
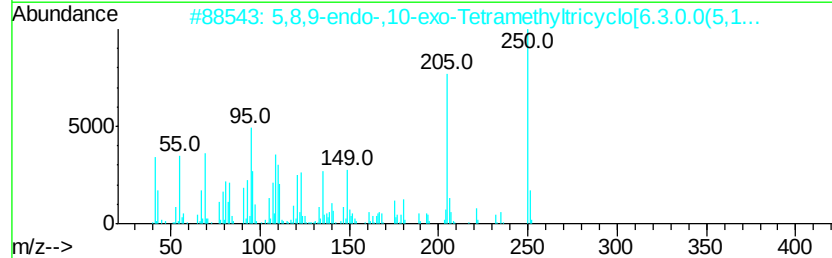
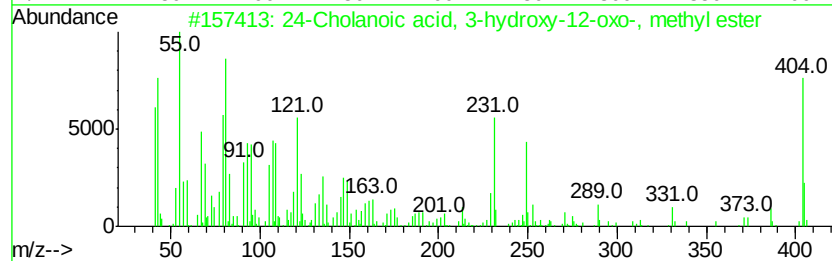
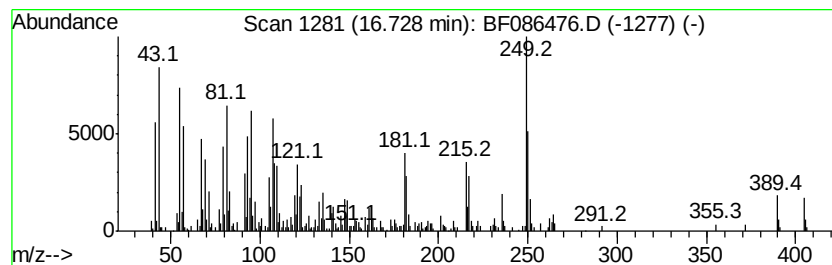
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown16.73 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.73	14.64 ng	651970	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	24-Cholanoic acid, 3-hydroxy-12-...	404	C25H40O4	028050-47-7	44
2		5,8,9-endo-,10-exo-Tetramethyltr...	250	C16H26O2	137235-57-5	30
3		1-[3-Fluoro-4-[4-(toluene-4-sulf...	404	C21H25FN2O3S	333751-65-8	30
4		Benzene, 1-nitro-2-hydroxy-4-(p-...	249	C12H8FN04	189214-56-0	22
5		Phenothiazin-4-ol, 8-chloro-	249	C12H8ClNOS	019807-55-7	18



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042816\
Data File : BF086476.D
Acq On : 28 Apr 2016 21:25
Operator : UM/SJ
Sample : H2654-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
26WARD-2A-CS-14(6-12FTBGS)

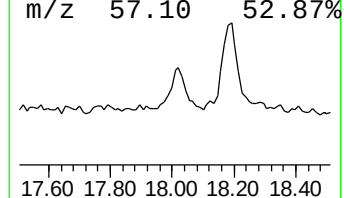
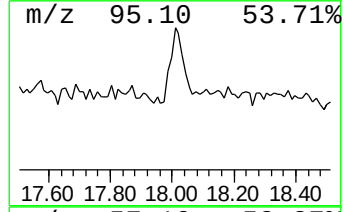
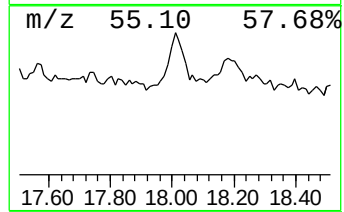
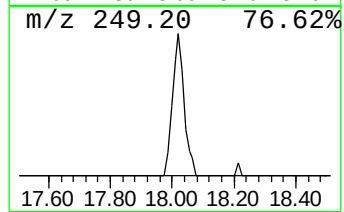
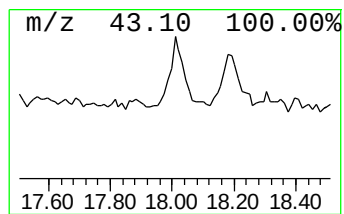
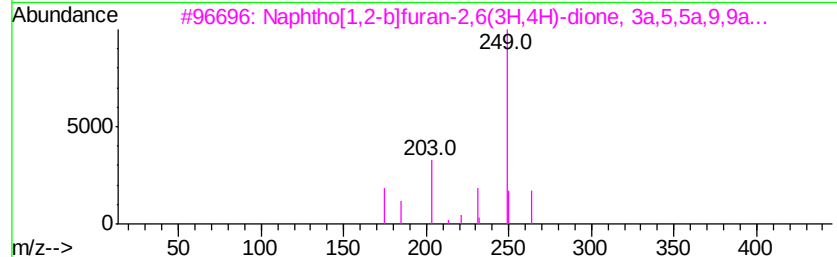
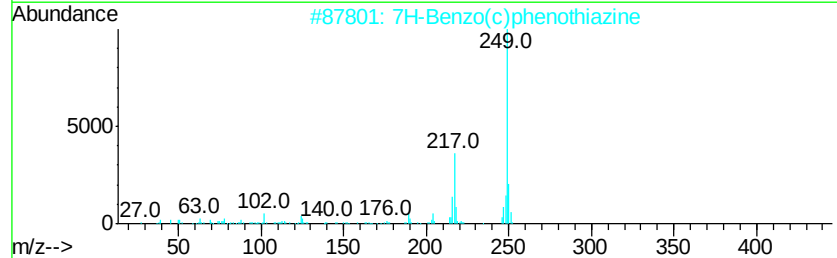
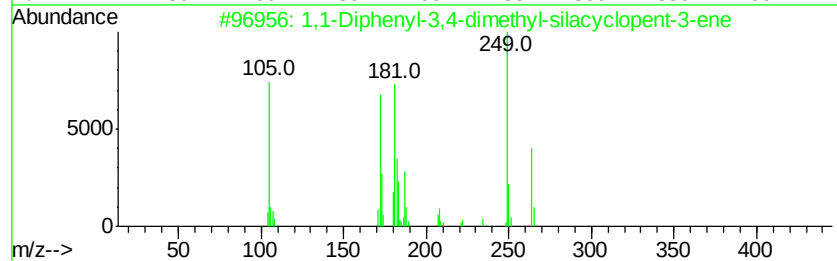
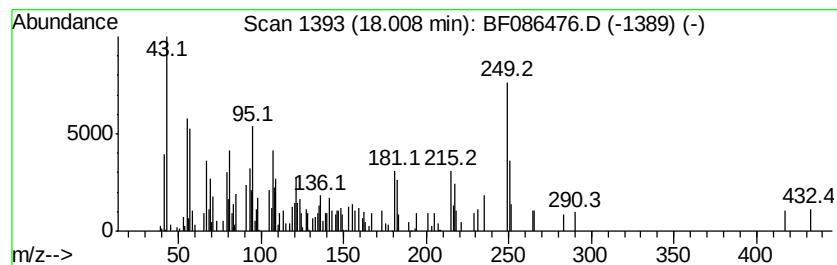
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown18.01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.01	3.78 ng	168605	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,1-Diphenyl-3,4-dimethyl-silacy...	264	C18H20Si	029163-98-2	32
2		7H-Benzo(c)phenothiazine	249	C16H11NS	000226-06-2	30
3		Naphtho[1,2-b]furan-2,6(3H,4H)-d...	264	C15H20O4	1000148-21-7	28
4		Etaqualone	264	C17H16N2O	007432-25-9	27
5		Methyl 6-methylthio-4[1H]quinolo...	249	C12H11N03S	1000255-48-3	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042816\
Data File : BF086476.D
Acq On : 28 Apr 2016 21:25
Operator : UM/SJ
Sample : H2654-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
26WARD-2A-CS-14(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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...	4.97	2.2	ng	116936	1	6.78	1058930	20.0
unknown6.56	6.56	79.1	ng	4187660	1	6.78	1058930	20.0
Hexadecane	10.26	2.4	ng	177660	3	9.82	1483760	20.0
Dodecane, 2-methy...	10.74	4.1	ng	257939	4	11.31	1268280	20.0
Trichloroacetic a...	13.79	8.3	ng	414776	5	13.94	1001520	20.0
Tetratriacontane	16.25	2.1	ng	94295	6	15.33	890974	20.0
unknown16.73	16.73	14.6	ng	651970	6	15.33	890974	20.0
unknown18.01	18.01	3.8	ng	168605	6	15.33	890974	20.0