

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100815\
 Data File : BF082125.D
 Acq On : 8 Oct 2015 13:42
 Operator : UM/IZ
 Sample : G3928-02
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OS-SB-22(22-24)

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-BF092815.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	5.040	251	254	269	rVB	647715	955736	39.90%	4.574%
2	5.463	288	291	293	rBV	1328723	1854214	77.40%	8.875%
3	6.492	378	381	384	rBV	1616979	1745828	72.88%	8.356%
4	6.629	390	393	395	rBV	2153960	2038041	85.08%	9.755%
5	6.857	411	413	416	rBV	342697	404707	16.89%	1.937%
6	7.017	425	427	429	rBV	1764320	1532899	63.99%	7.337%
7	7.429	461	463	470	rBV	1139290	1164316	48.60%	5.573%
8	8.149	524	526	528	rBV	637535	560891	23.41%	2.685%
9	8.960	595	597	601	rBB	33590	31168	1.30%	0.149%
10	9.223	618	620	623	rBV	1979357	2075478	86.64%	9.934%
11	9.623	653	655	657	rBV	409369	352813	14.73%	1.689%
12	9.909	677	680	681	rBV	524297	664125	27.72%	3.179%
13	9.932	681	682	685	rVB	29432	29330	1.22%	0.140%
14	10.320	713	716	719	rBV	51652	56789	2.37%	0.272%
15	10.698	746	749	751	rBV	1440140	1588370	66.30%	7.602%
16	10.801	757	758	765	rVB	16169	28245	1.18%	0.135%
17	11.395	807	810	812	rBV	511788	689823	28.80%	3.302%
18	11.612	827	829	833	rBV	32717	52614	2.20%	0.252%
19	11.921	852	856	857	rBV	55612	64594	2.70%	0.309%
20	12.435	899	901	909	rBV	196597	332155	13.87%	1.590%
21	12.789	931	932	934	rBV	65400	84647	3.53%	0.405%
22	12.835	934	936	938	rBV2	21148	31472	1.31%	0.151%
23	12.984	946	949	951	rBV	2004763	2395556	100.00%	11.466%
24	13.418	985	987	989	rBV	64828	55594	2.32%	0.266%
25	13.498	992	994	996	rVV2	68509	69281	2.89%	0.332%
26	13.875	1025	1027	1034	rBV	48535	80292	3.35%	0.384%
27	14.035	1038	1041	1043	rVV	465444	625509	26.11%	2.994%
28	14.492	1077	1081	1084	rBV2	24721	30869	1.29%	0.148%
29	14.790	1104	1107	1110	rBV2	22904	43411	1.81%	0.208%
30	14.870	1110	1114	1116	rVB2	39574	66713	2.78%	0.319%
31	15.258	1146	1148	1153	rBV	39883	63678	2.66%	0.305%
32	15.475	1164	1167	1175	rBV	403421	572413	23.89%	2.740%
33	15.738	1187	1190	1193	rVB	66817	112914	4.71%	0.540%
34	16.287	1234	1238	1245	rVB	56866	121858	5.09%	0.583%

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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 >
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35	16.961	1289	1297	1303	rBV2	43426	116507	4.86%	0.558%
36	17.773	1363	1368	1376	rVB2	26804	81039	3.38%	0.388%
37	18.778	1449	1456	1462	rVB2	16510	62386	2.60%	0.299%
38	20.024	1556	1565	1575	rVB4	10767	56537	2.36%	0.271%

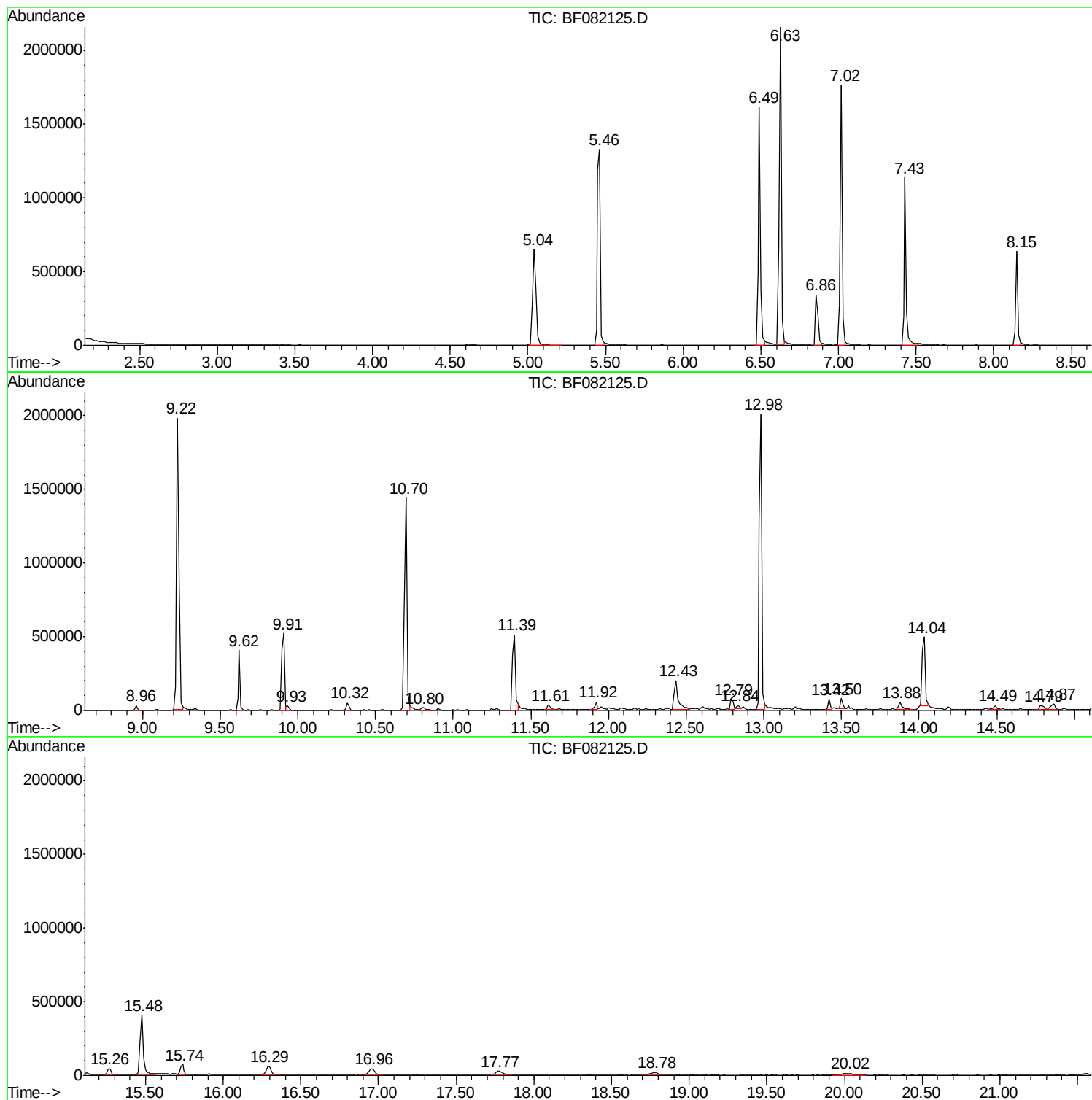
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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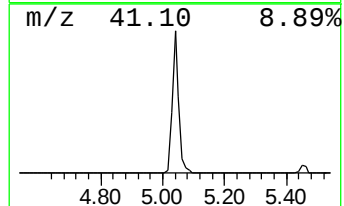
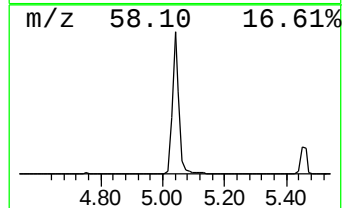
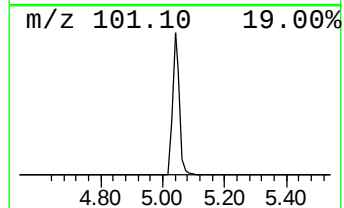
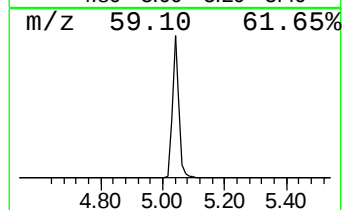
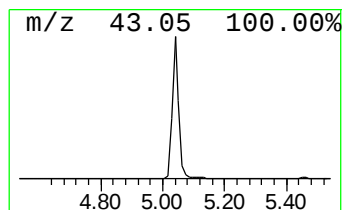
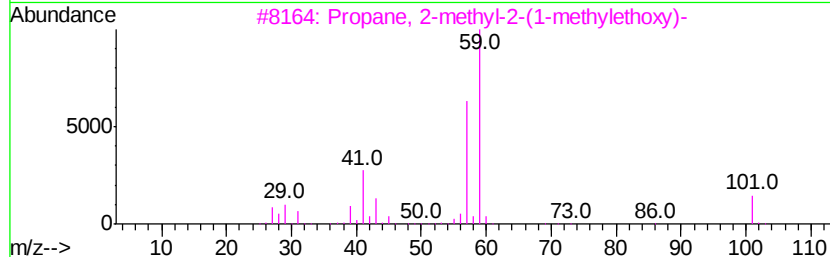
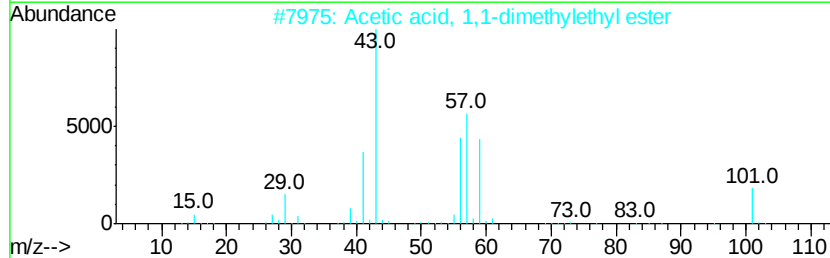
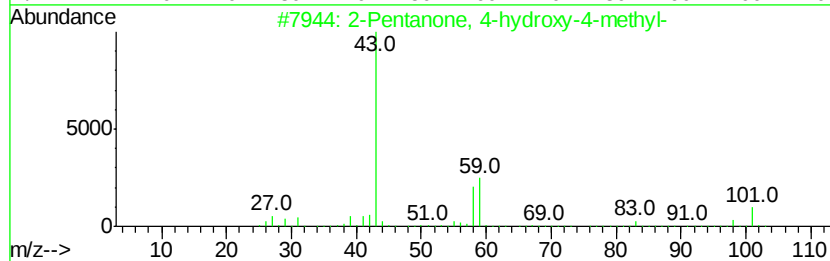
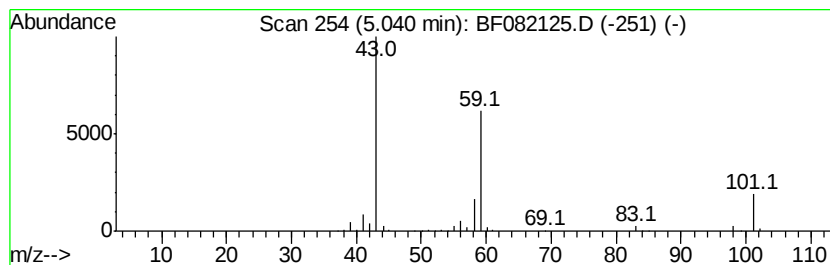
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	47.23 ng	955736	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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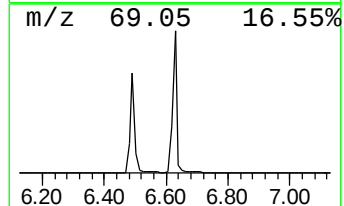
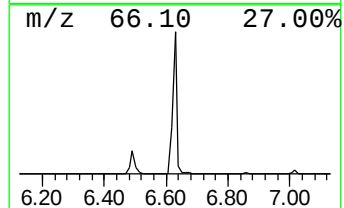
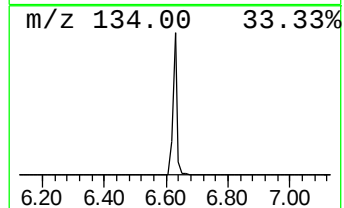
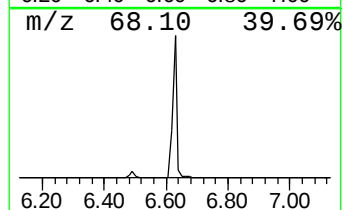
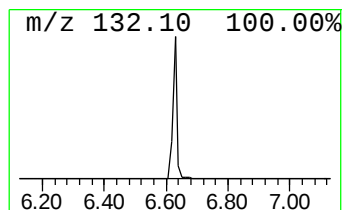
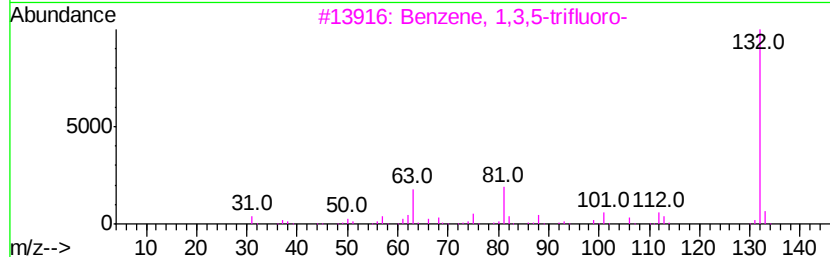
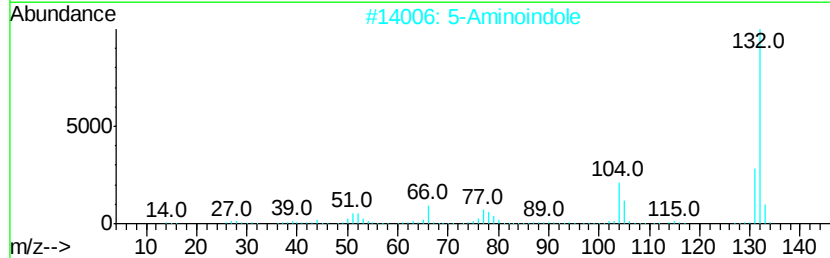
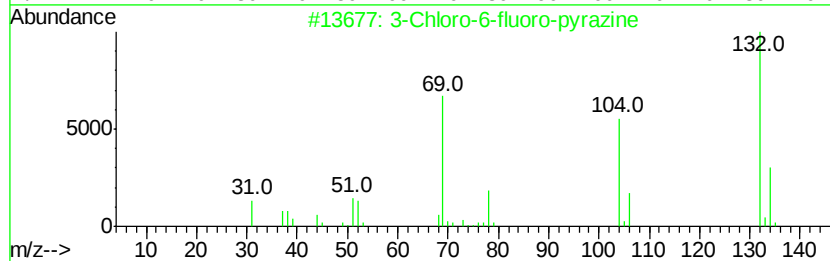
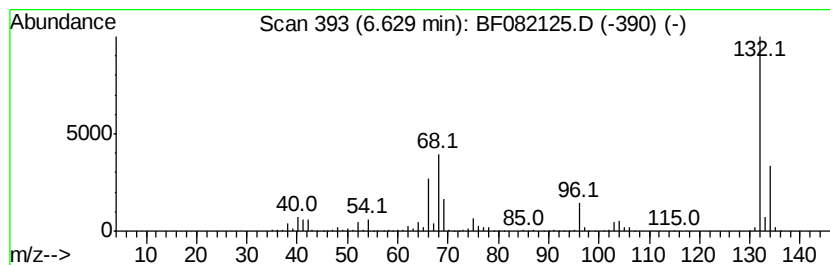
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Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	100.72 ng	2038040	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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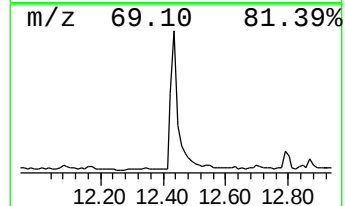
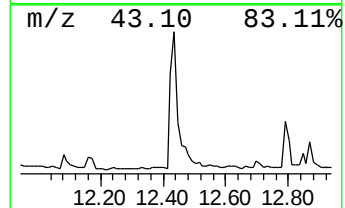
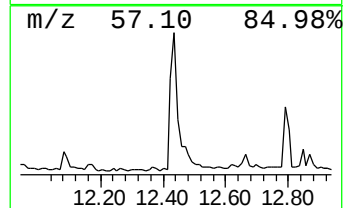
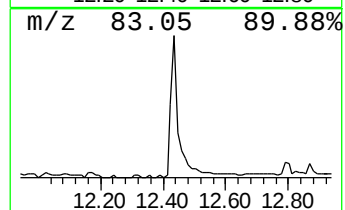
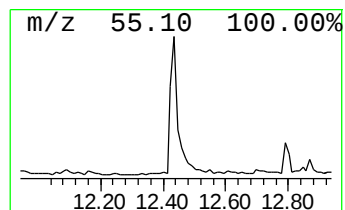
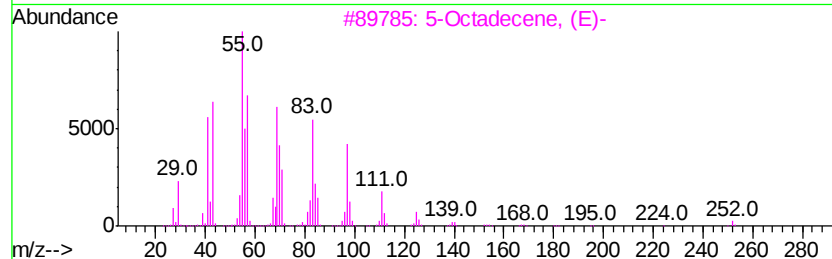
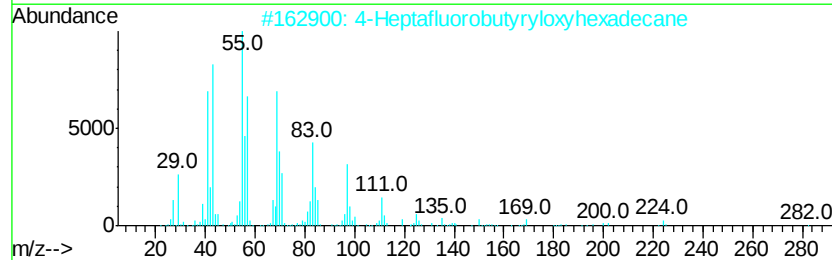
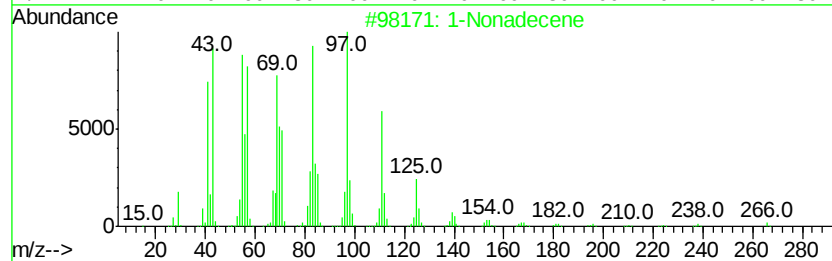
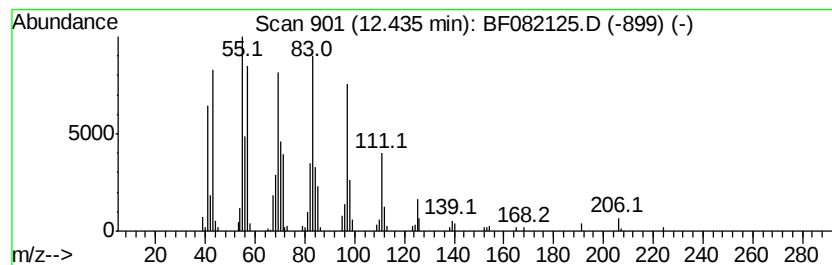
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Nonadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.44	9.63 ng	332155	Phenanthrene-d10	11.39		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene		266	C19H38	018435-45-5	91
2	4-Heptafluorobutyryloxyhexadecane		438	C20H33F7O2	1000282-97-2	91
3	5-Octadecene, (E)-		252	C18H36	007206-21-5	91
4	Bromoacetic acid, hexadecyl ester		362	C18H35BrO2	005454-48-8	91
5	Bromoacetic acid, pentadecyl ester		348	C17H33BrO2	131143-01-6	91



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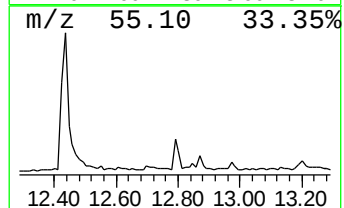
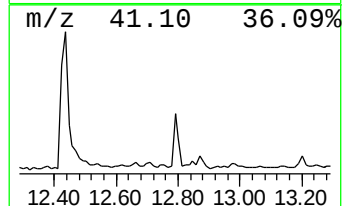
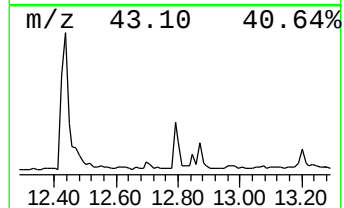
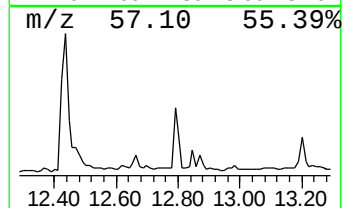
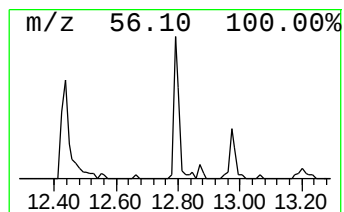
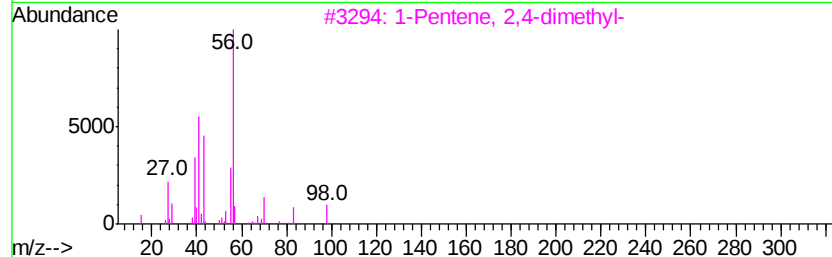
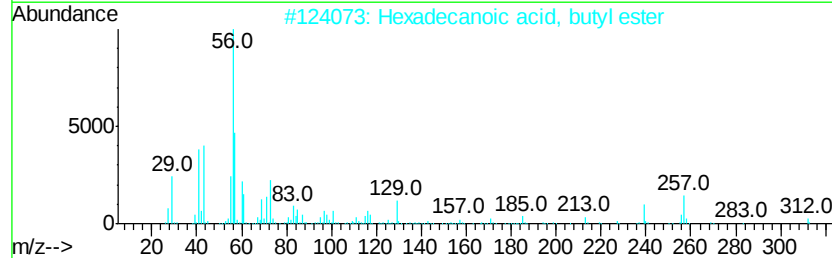
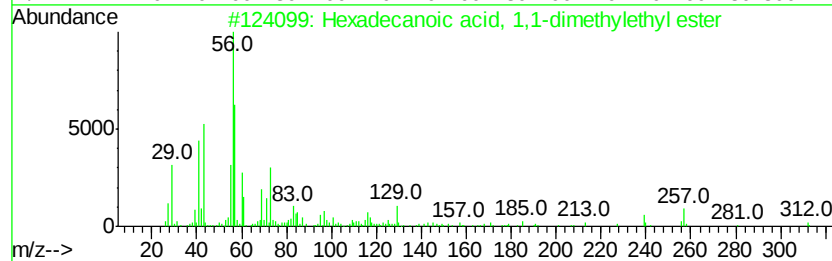
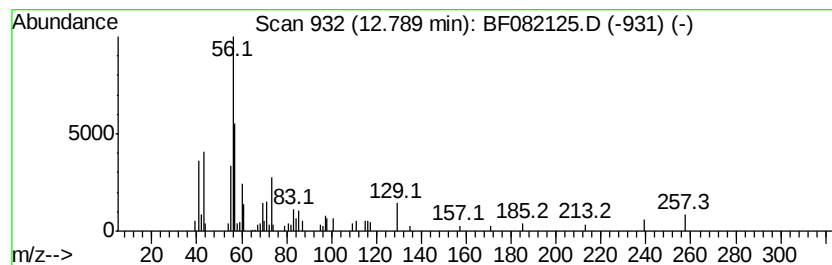
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Hexadecanoic acid, 1,1-dime... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	2.71 ng	84647	Chrysene-d12	14.04

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	91
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
3		1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	38
4		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	37
5		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	37



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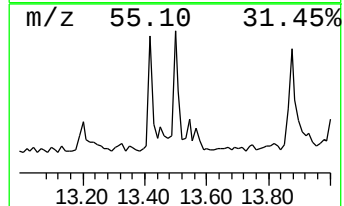
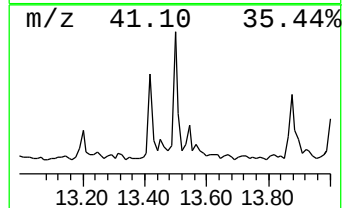
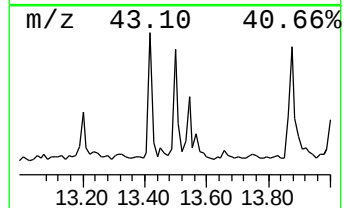
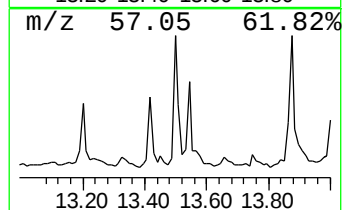
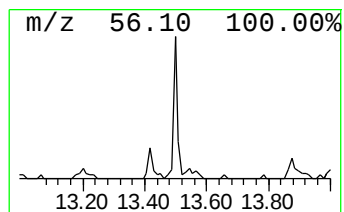
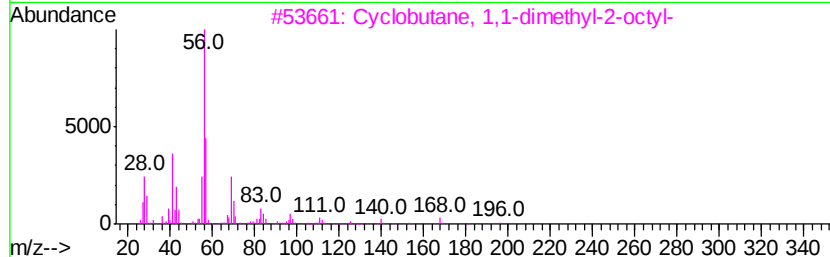
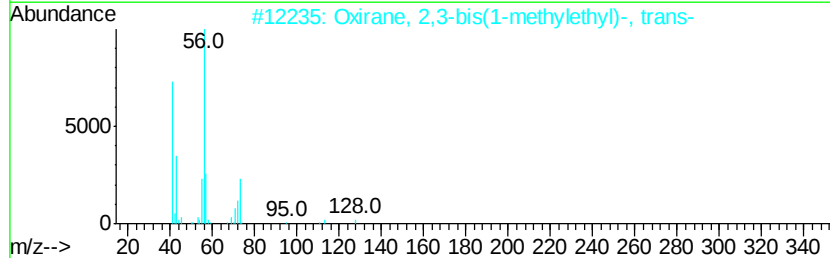
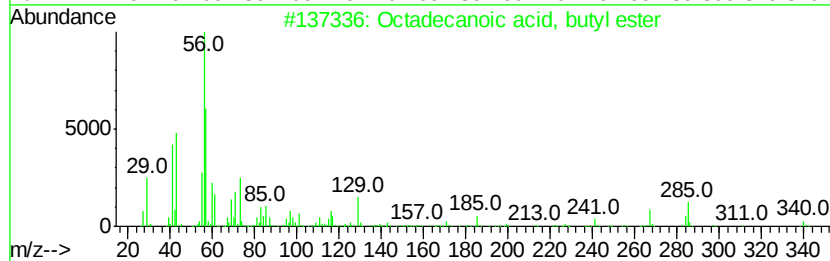
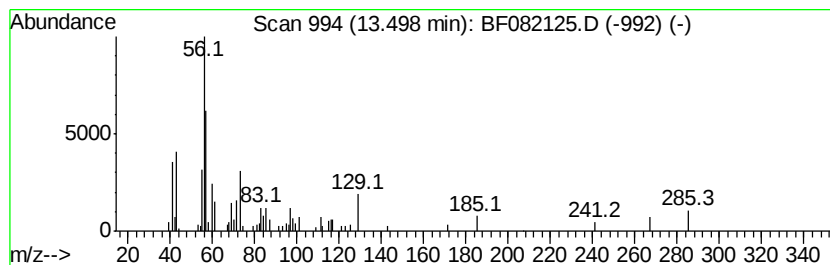
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	2.22 ng	69281	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	38
3		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
4		2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35
5		Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100815\
Data File : BF082125.D
Acq On : 8 Oct 2015 13:42
Operator : UM/IZ
Sample : G3928-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
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ClientSampleId :
OS-SB-22(22-24)

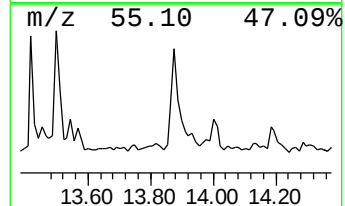
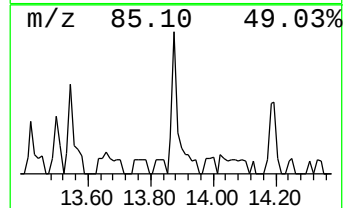
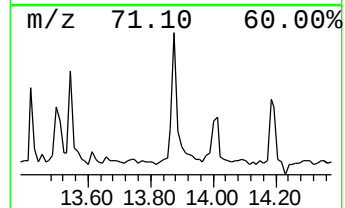
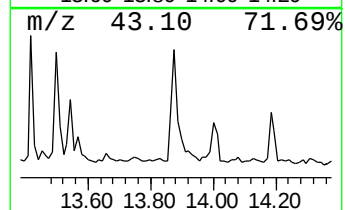
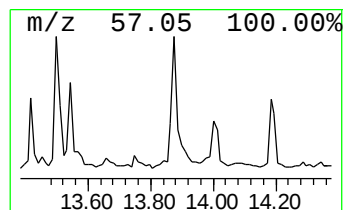
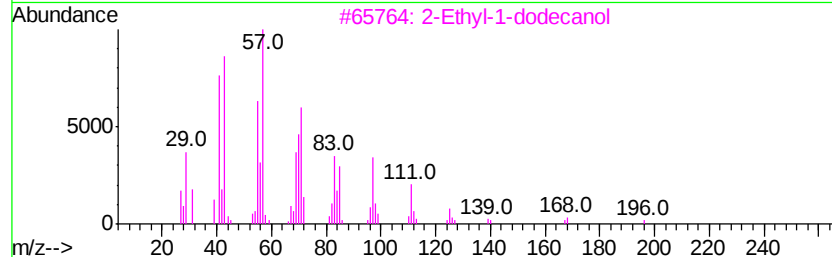
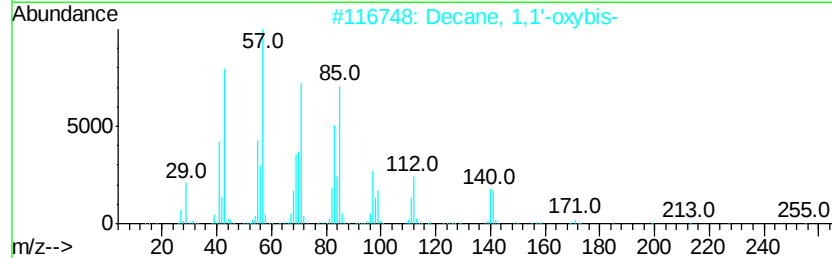
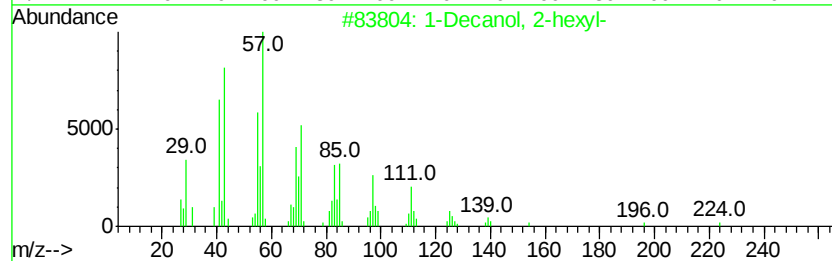
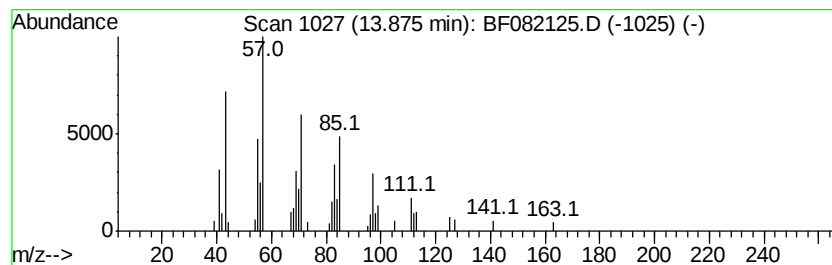
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Decanol, 2-hexyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	2.57 ng	80292	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	83
2		Decane, 1,1'-oxybis-	298	C20H42O	002456-28-2	80
3		2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	72
4		Tetratetracontane	619	C44H90	007098-22-8	59
5		Heptacosane	380	C27H56	000593-49-7	53



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100815\
Data File : BF082125.D
Acq On : 8 Oct 2015 13:42
Operator : UM/IZ
Sample : G3928-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OS-SB-22(22-24)

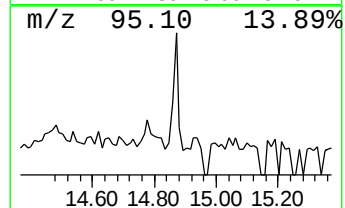
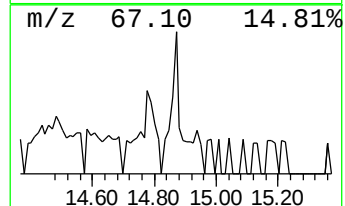
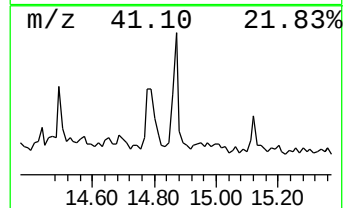
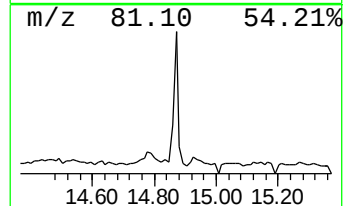
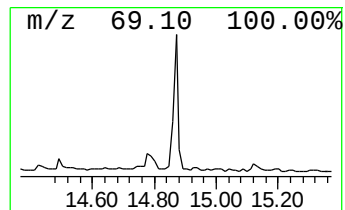
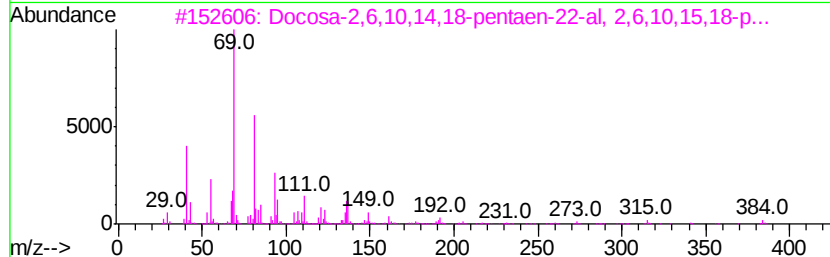
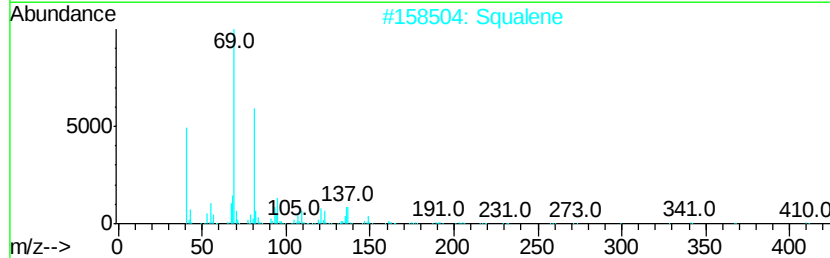
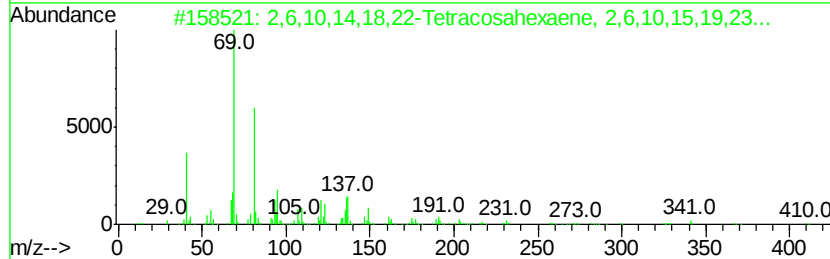
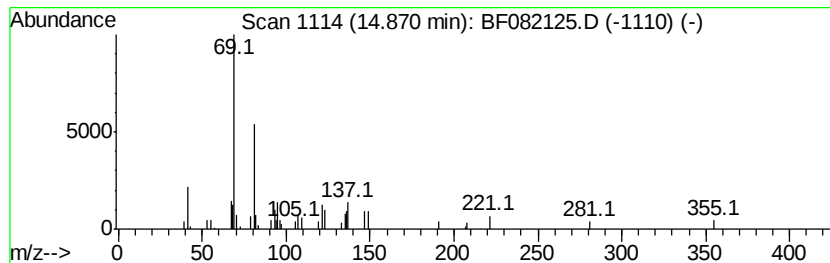
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2,6,10,14,18,22-Tetracosahexaene... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	2.33 ng	66713	Perylene-d12	15.48

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	83		
2	Squalene	410	C30H50	007683-64-9	72		
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	72		
4	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	72		
5	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	59		



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100815\
Data File : BF082125.D
Acq On : 8 Oct 2015 13:42
Operator : UM/IZ
Sample : G3928-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
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ClientSampleId :
OS-SB-22(22-24)

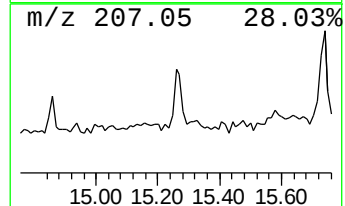
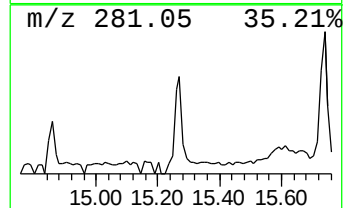
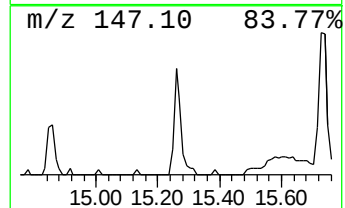
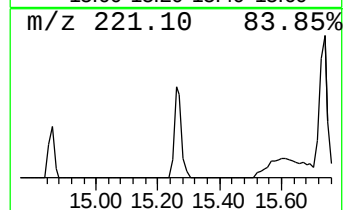
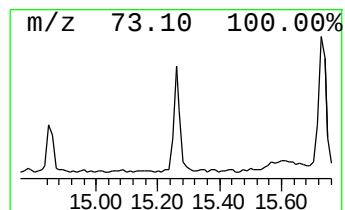
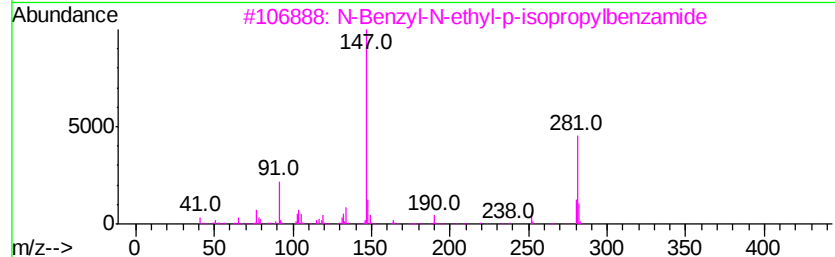
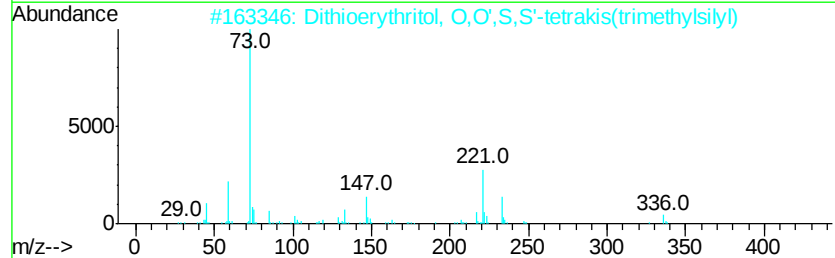
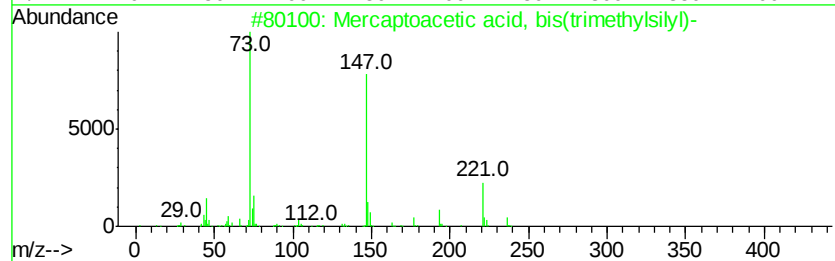
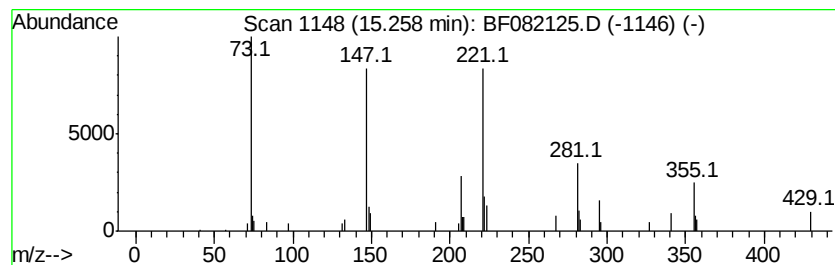
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown15.26 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.26	2.22 ng	63678	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	38
2		Dithioerythritol, O,O',S,S'-tetr...	442	C16H42O2S2Si4	1000079-30-7	32
3		N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	27
4		1,2-Benzenedicarboxylic acid, bi...	310	C14H22O4Si2	002078-22-0	22
5		1,3-Benzodioxole, 5-[3-acetamino...	221	C12H15NO3	1000124-33-0	22



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100815\
Data File : BF082125.D
Acq On : 8 Oct 2015 13:42
Operator : UM/IZ
Sample : G3928-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
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ClientSampleId :
OS-SB-22(22-24)

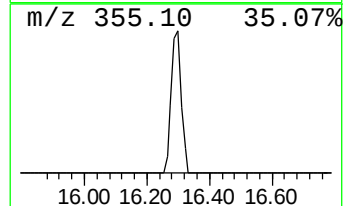
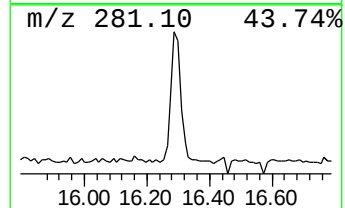
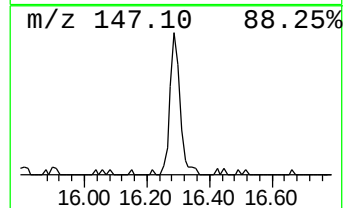
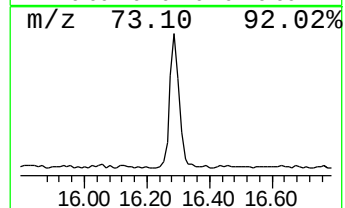
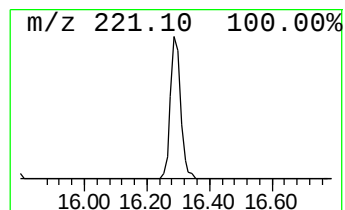
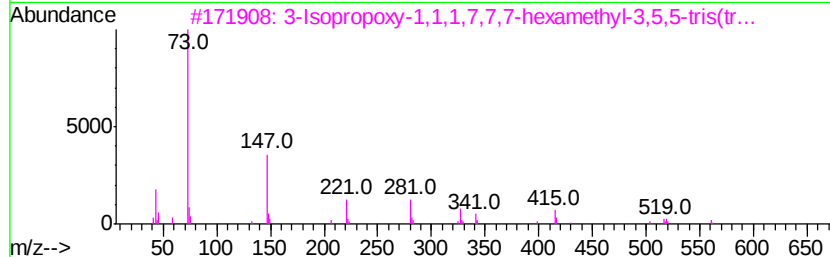
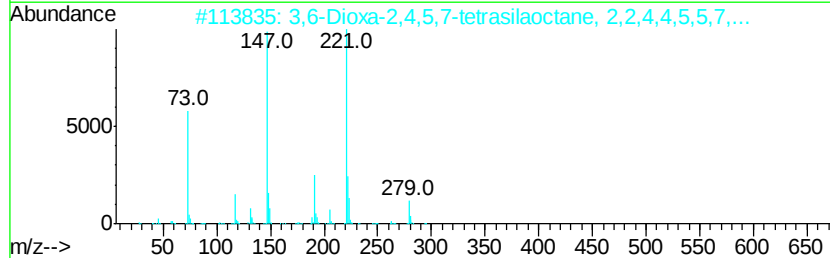
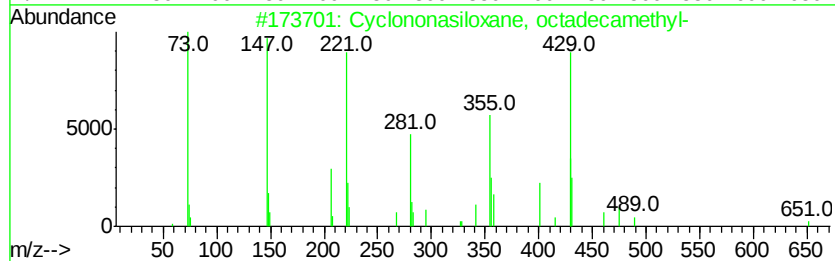
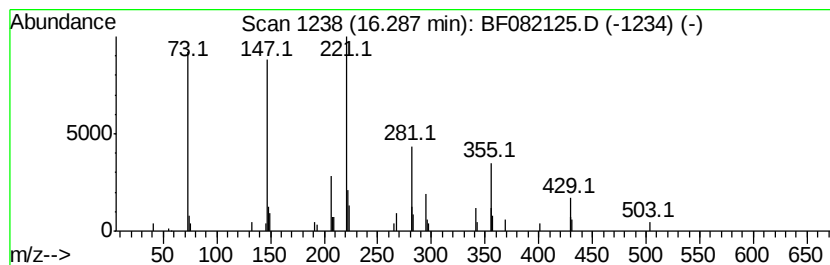
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown16.29 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.29	4.26 ng	121858	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	68
2		3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	40
3		3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	38
4		Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	38
5		1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100815\
Data File : BF082125.D
Acq On : 8 Oct 2015 13:42
Operator : UM/IZ
Sample : G3928-02
Misc :
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Instrument :
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ClientSampleId :
OS-SB-22(22-24)

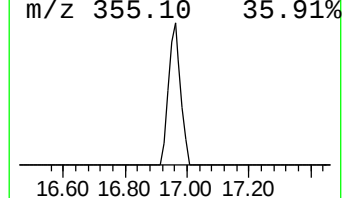
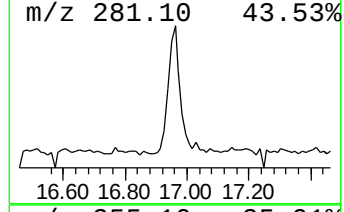
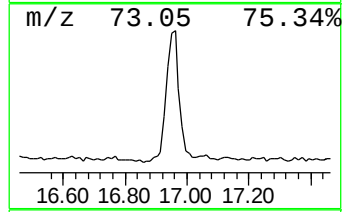
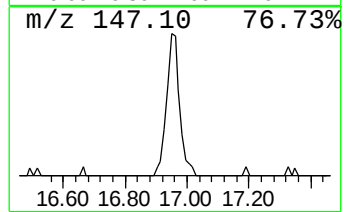
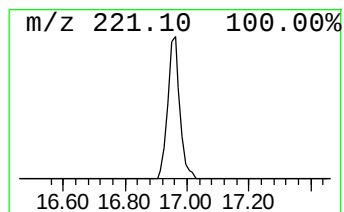
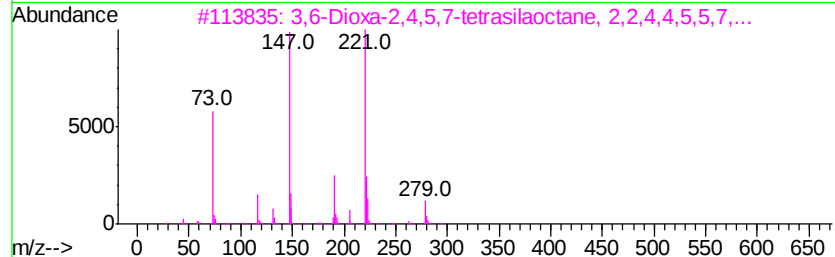
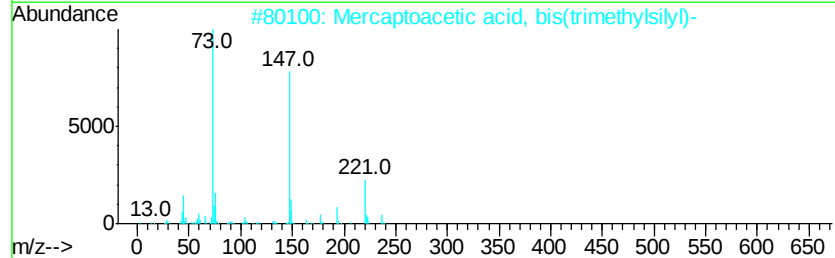
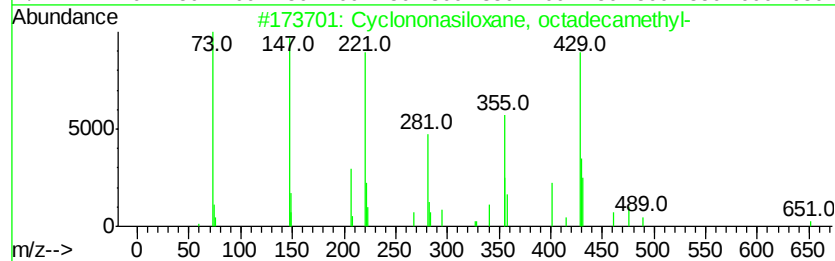
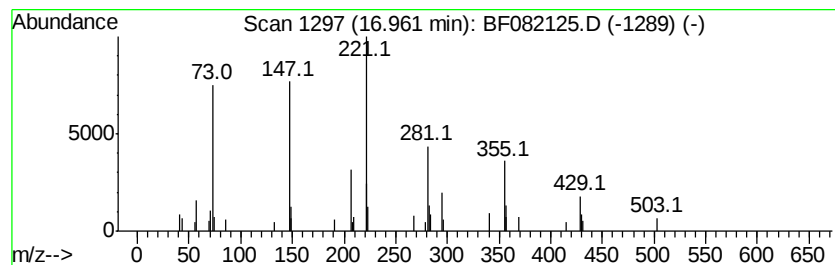
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown16.96 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.96	4.07 ng	116507	Perylene-d12	15.48

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H5409Si9	000556-71-8	90
2			Mercaptoacetic acid, bis(trimeth...	236	C8H2002SSi2	006398-62-5	47
3			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H3002Si4	004342-25-0	40
4			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H4005Si6	038147-00-1	37
5			2-(2',4',4',6',6',8',8'-Heptamet...	652	C16H48010Si9	145344-72-5	32



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100815\
Data File : BF082125.D
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Operator : UM/IZ
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Misc :
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ClientSampleId :
OS-SB-22(22-24)

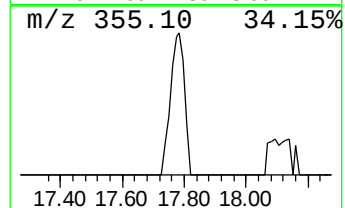
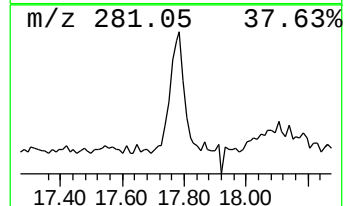
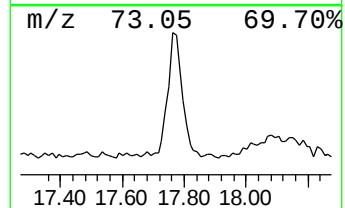
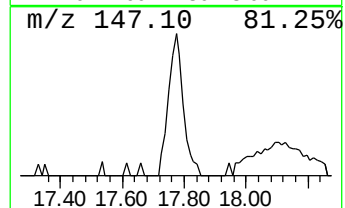
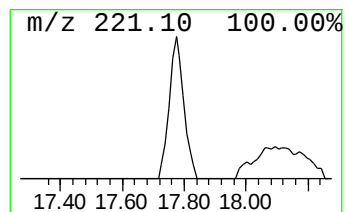
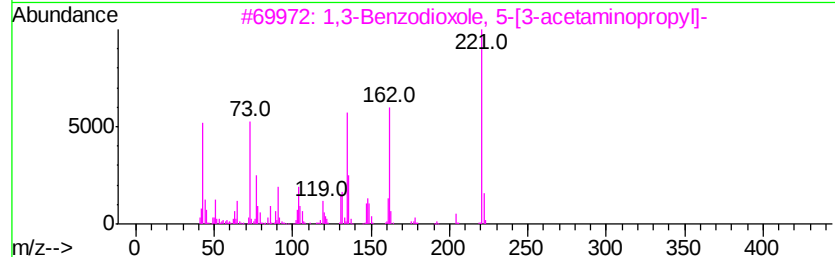
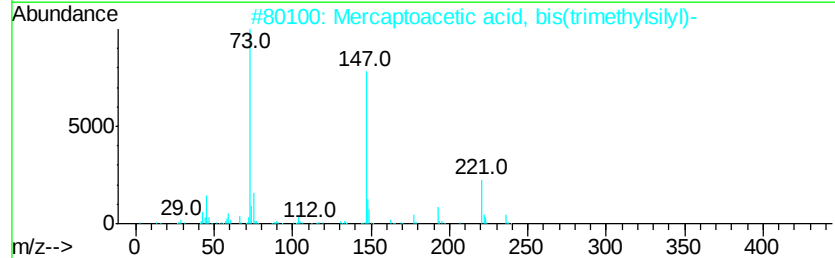
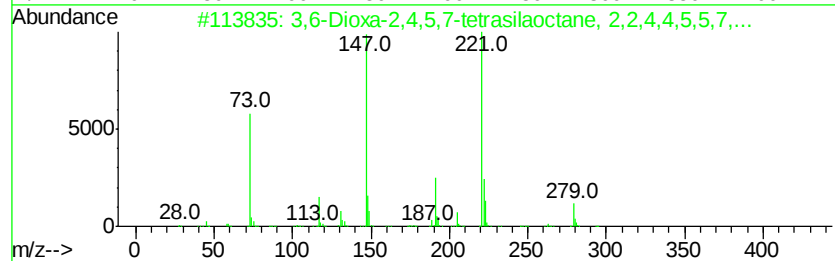
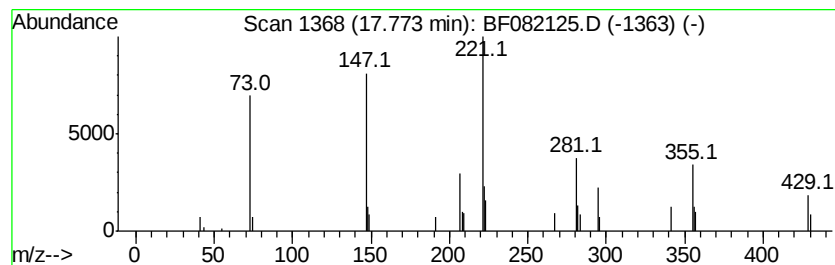
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown17.77 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.77	2.83 ng	81039	Perylene-d12	15.48

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	50
2			Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	40
3			1,3-Benzodioxole, 5-[3-acetamino...	221	C12H15NO3	1000124-33-0	27
4			2-(2',4',4',6',6',8',8'-Heptamet...	652	C16H48O10Si9	145344-72-5	25
5			3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100815\
Data File : BF082125.D
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Misc :
ALS Vial : 26 Sample Multiplier: 1

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ClientSampleId :
OS-SB-22(22-24)

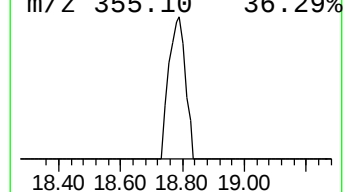
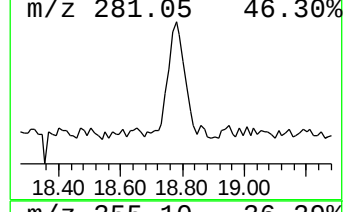
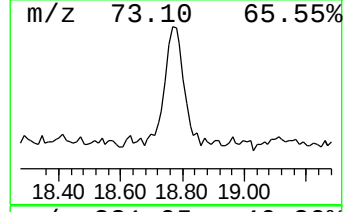
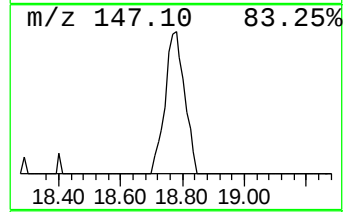
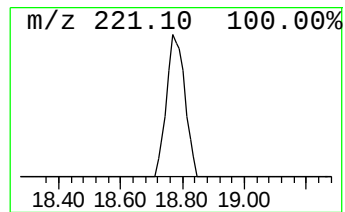
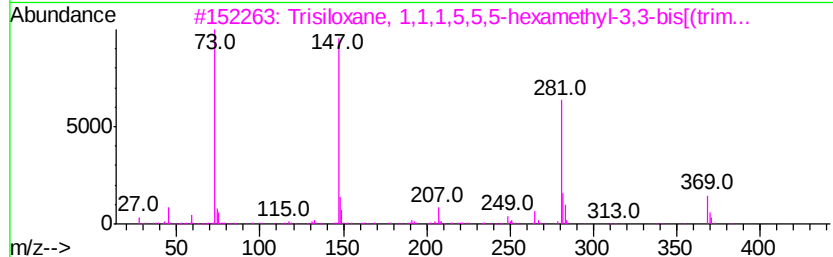
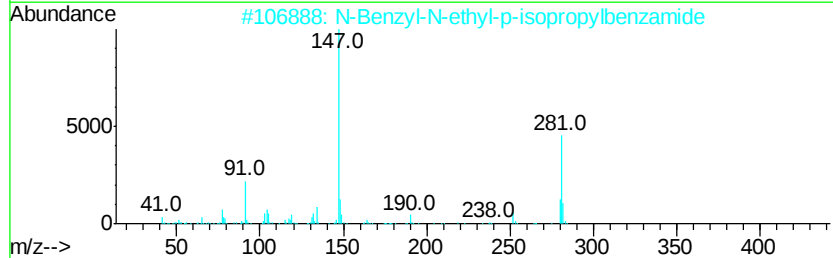
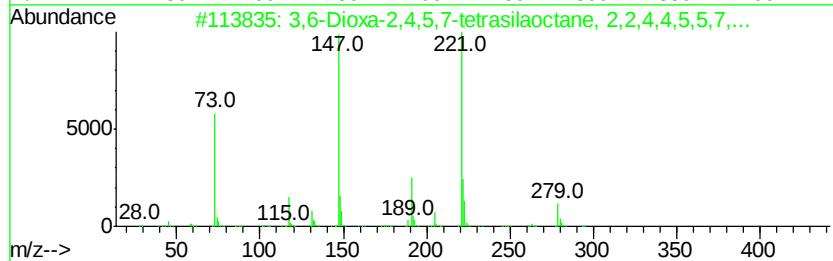
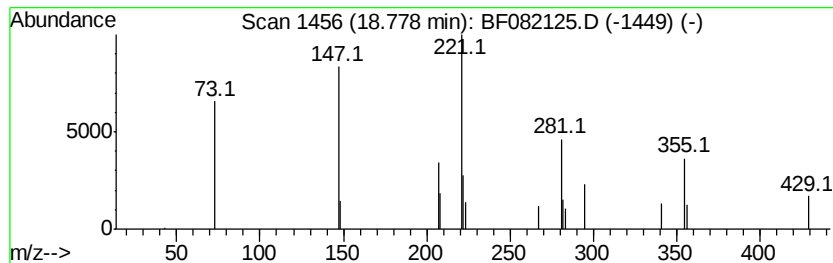
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown18.78 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.78	2.18 ng	62386	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H3002Si4	004342-25-0	47
2		N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	27
3		Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H3604Si5	003555-47-3	27
4		Pentasiloxane, dodecamethyl-	384	C12H3604Si5	000141-63-9	16
5		Trisiloxane, octamethyl-	236	C8H2402Si3	000107-51-7	12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100815\
 Data File : BF082125.D
 Acq On : 8 Oct 2015 13:42
 Operator : UM/IZ
 Sample : G3928-02
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OS-SB-22(22-24)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.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...	5.04	47.2	ng	955736	1	6.86	404707	20.0
unknown6.63	6.63	100.7	ng	2038040	1	6.86	404707	20.0
1-Nonadecene	12.44	9.6	ng	332155	4	11.39	689823	20.0
Hexadecanoic acid...	12.79	2.7	ng	84647	5	14.04	625509	20.0
Octadecanoic acid...	13.50	2.2	ng	69281	5	14.04	625509	20.0
1-Decanol, 2-hexyl-	13.88	2.6	ng	80292	5	14.04	625509	20.0
2,6,10,14,18,22-T...	14.87	2.3	ng	66713	6	15.48	572413	20.0
unknown15.26	15.26	2.2	ng	63678	6	15.48	572413	20.0
unknown16.29	16.29	4.3	ng	121858	6	15.48	572413	20.0
unknown16.96	16.96	4.1	ng	116507	6	15.48	572413	20.0
unknown17.77	17.77	2.8	ng	81039	6	15.48	572413	20.0
unknown18.78	18.78	2.2	ng	62386	6	15.48	572413	20.0