

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF111217\
 Data File : BF100490.D
 Acq On : 12 Nov 2017 15:27
 Operator : SJ/JU
 Sample : I6403-03
 Misc :
 ALS Vial : 59 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 110817-JETT-F-U-B

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-BF110817.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	2.199	15	19	25	rVB	82467	109584	2.65%	0.446%
2	5.116	512	515	526	rBV	269178	282826	6.83%	1.150%
3	5.516	578	583	586	rBV	1327526	1274143	30.77%	5.182%
4	6.516	749	753	757	rBV	969367	850726	20.55%	3.460%
5	6.669	774	779	782	rBV	2475339	2246898	54.26%	9.139%
6	6.898	815	818	822	rBV	989581	822855	19.87%	3.347%
7	7.057	841	845	849	rVB	3023231	3012013	72.74%	12.251%
8	7.463	909	914	917	rBV	2322016	2542981	61.41%	10.343%
9	8.181	1032	1036	1040	rBV	1257577	1023194	24.71%	4.162%
10	9.257	1214	1219	1223	rBV	3975086	4140697	100.00%	16.842%
11	9.645	1282	1285	1293	rVB	152972	122855	2.97%	0.500%
12	9.886	1323	1326	1329	rBV2	341101	322221	7.78%	1.311%
13	9.939	1329	1335	1349	rVB	1082454	1069719	25.83%	4.351%
14	10.645	1452	1455	1460	rVB	55932	49627	1.20%	0.202%
15	10.722	1464	1468	1480	rBV	1411038	1394463	33.68%	5.672%
16	11.422	1583	1587	1591	rBV	983730	828956	20.02%	3.372%
17	12.822	1822	1825	1828	rVB	120895	87812	2.12%	0.357%
18	13.010	1852	1857	1860	rBV	3225413	3038458	73.38%	12.359%
19	13.527	1941	1945	1948	rBV	76568	59438	1.44%	0.242%
20	14.063	2032	2036	2045	rVB	803294	761204	18.38%	3.096%
21	15.545	2282	2288	2299	rBV	383298	545060	13.16%	2.217%

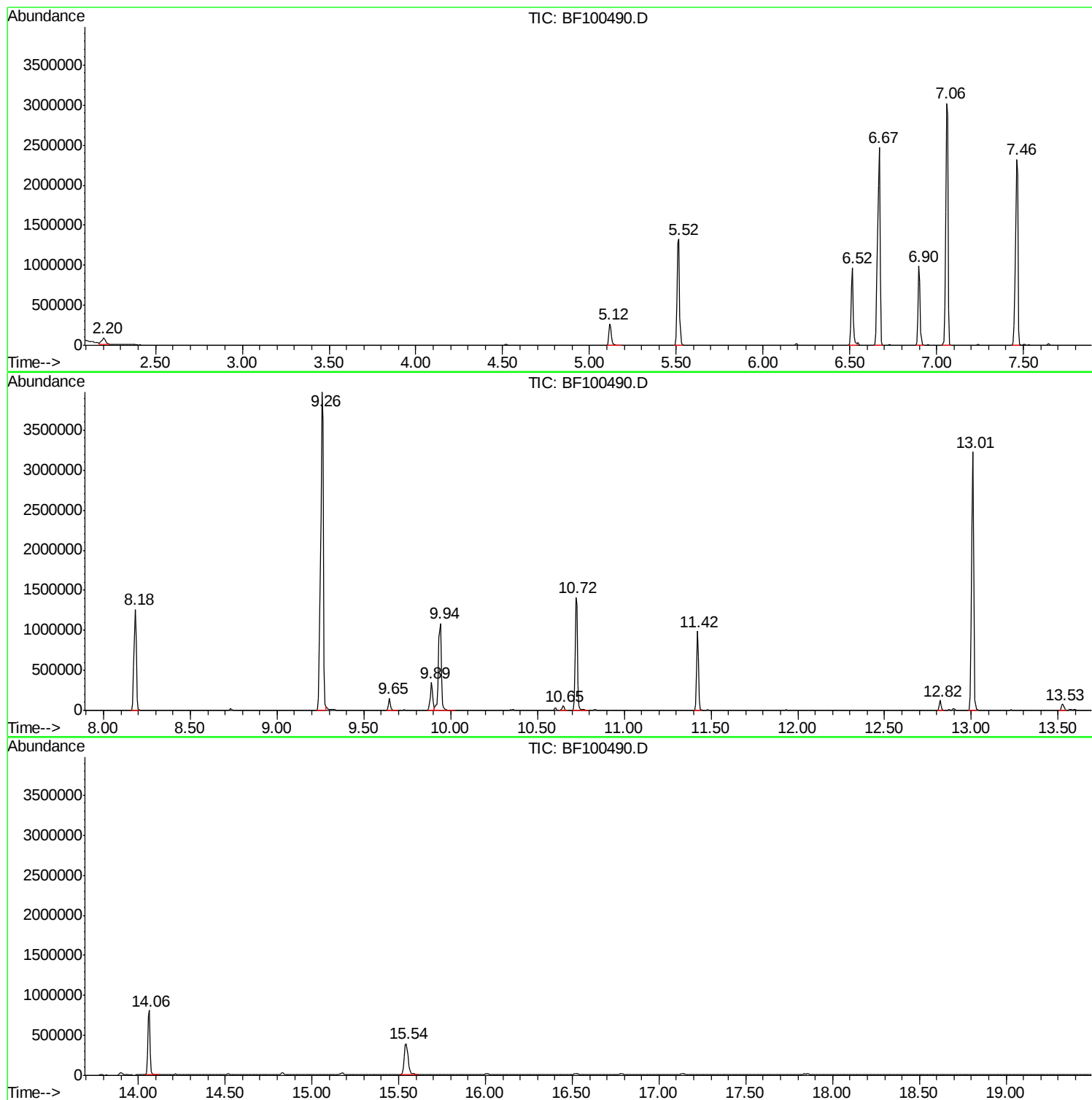
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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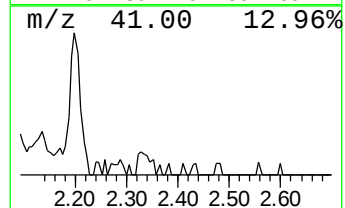
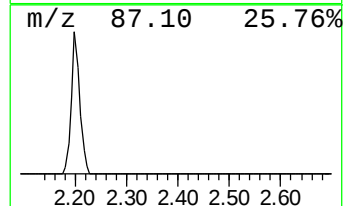
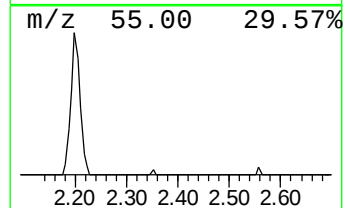
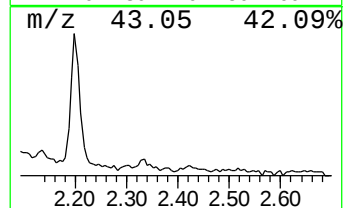
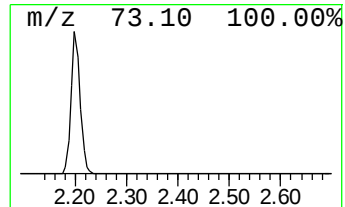
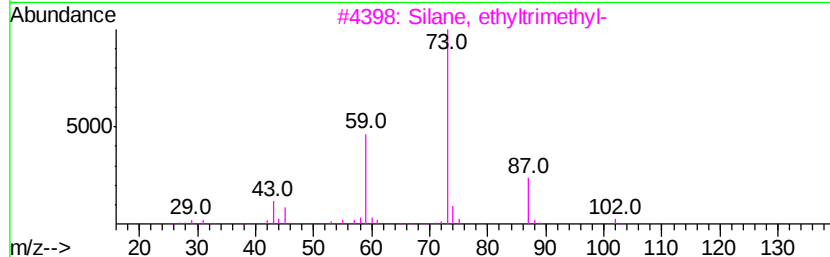
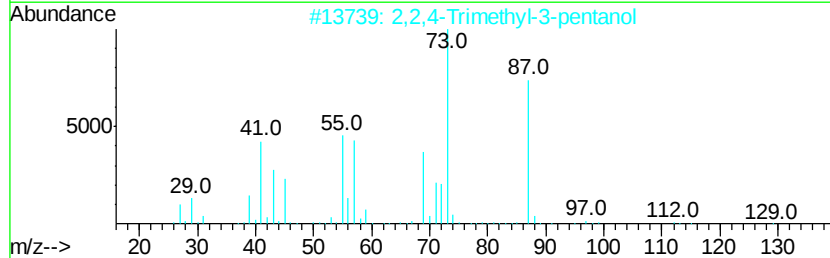
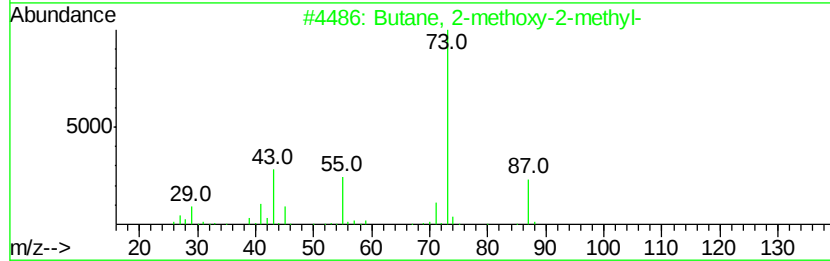
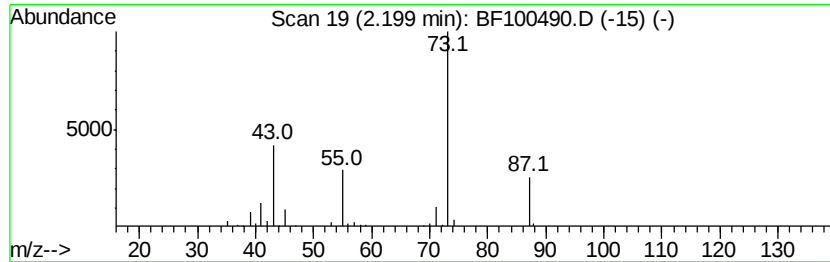
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	2.66 ng	109584	1,4-Dichlorobenzene-d4	6.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
5			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	23



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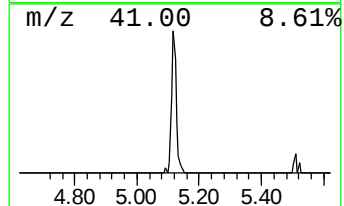
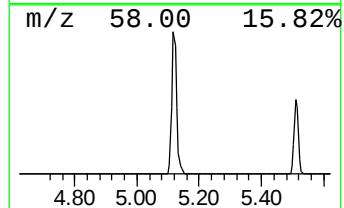
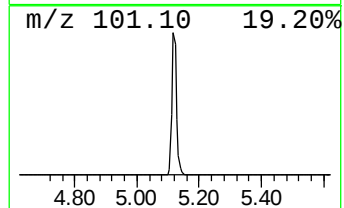
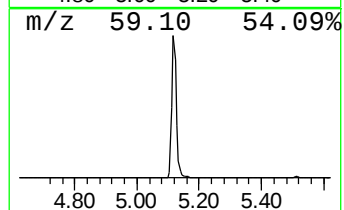
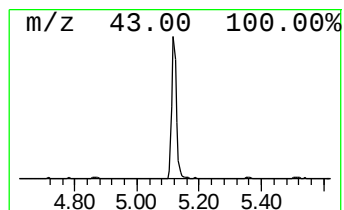
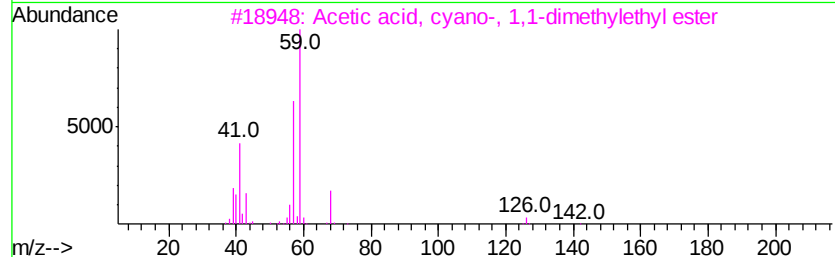
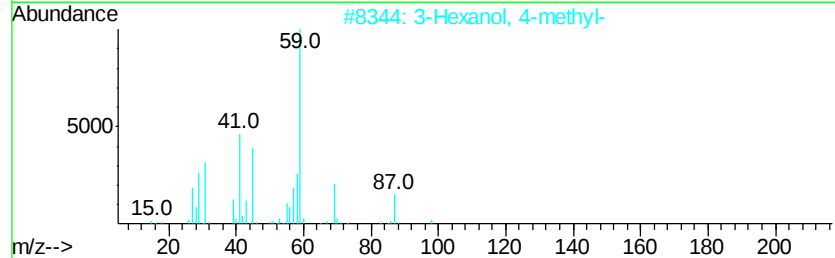
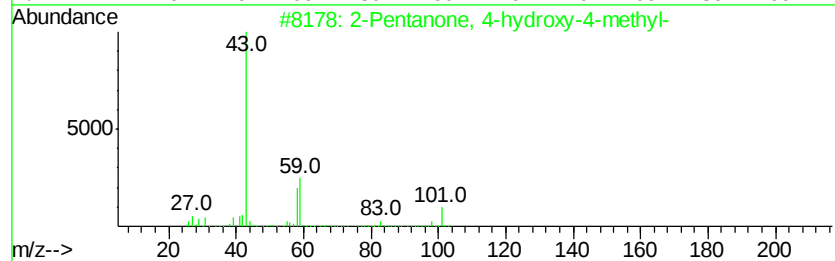
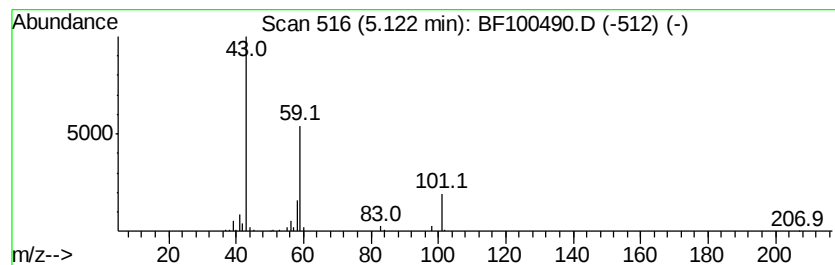
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	6.87 ng	282826	1,4-Dichlorobenzene-d4	6.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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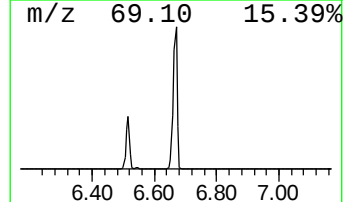
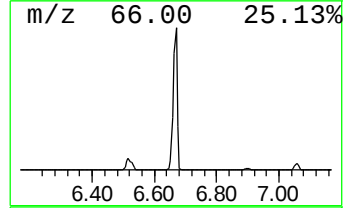
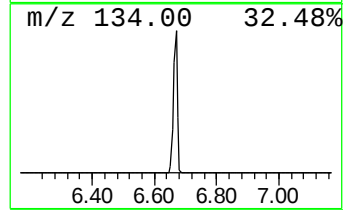
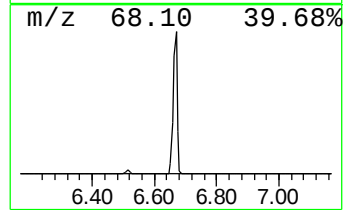
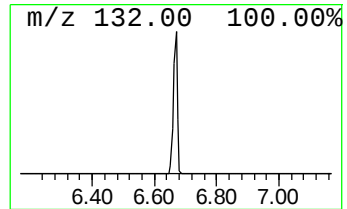
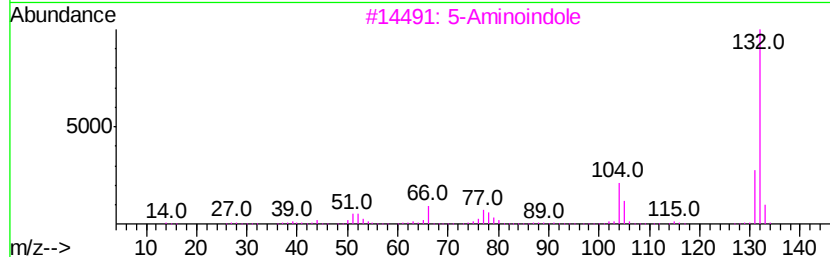
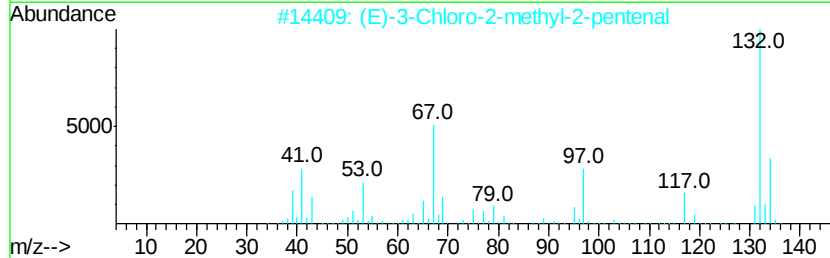
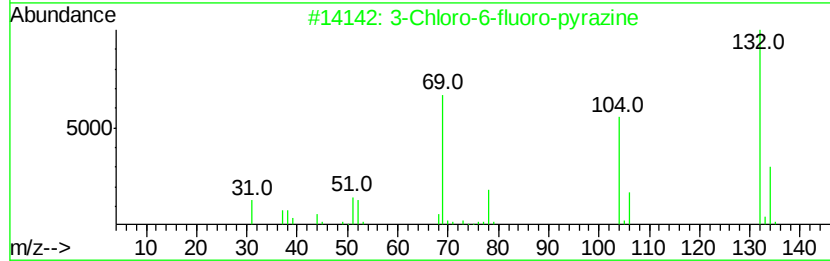
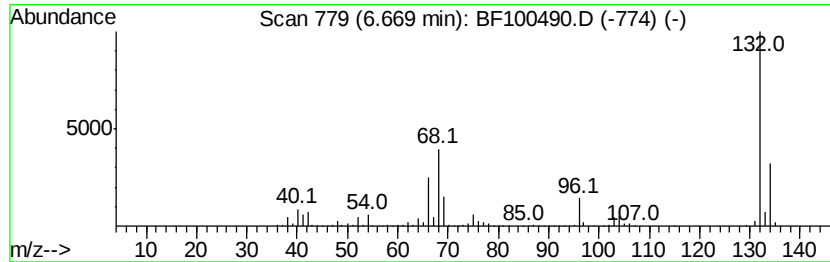
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.67 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	54.61 ng	2246900	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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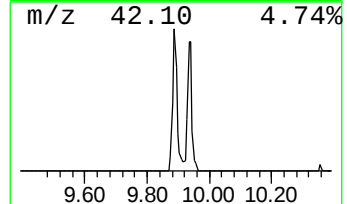
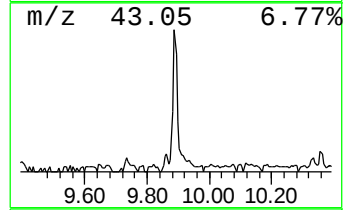
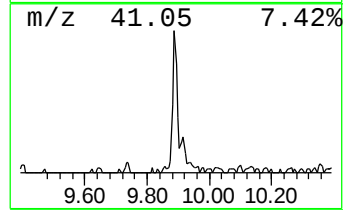
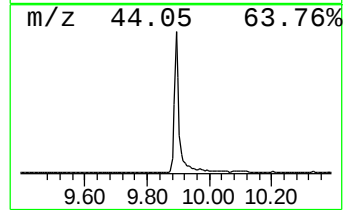
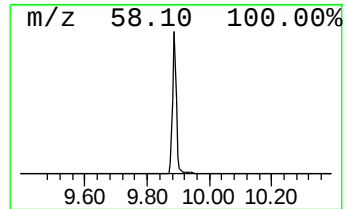
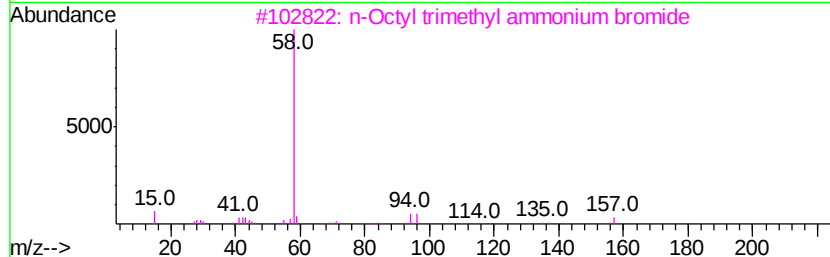
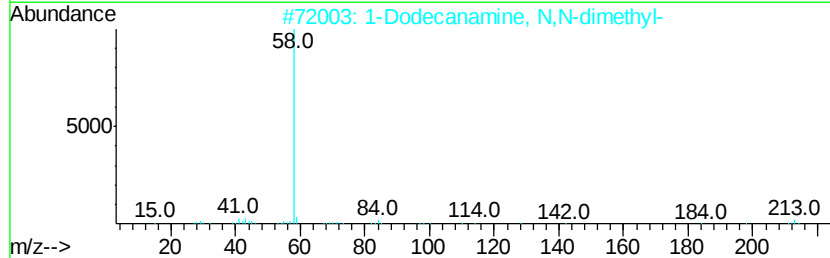
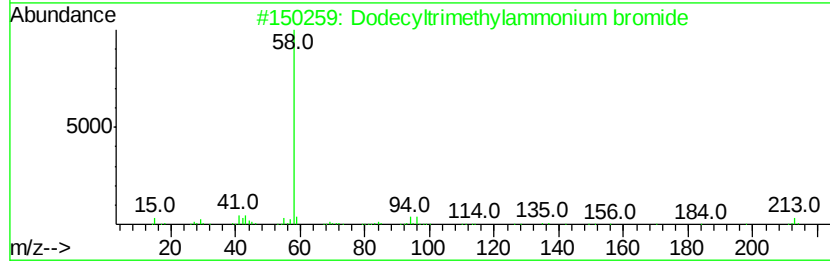
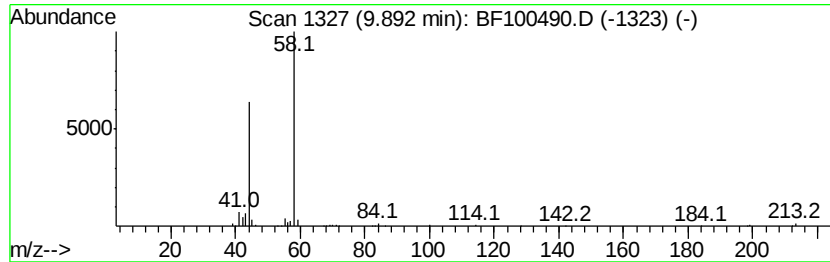
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Peak Number 5 Dodecyltrimethylammonium br... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.89	6.02 ng	322221	Acenaphthene-d10	9.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecyltrimethylammonium bromide	307	C15H34BrN	001119-94-4	72
2		1-Dodecanamine, N,N-dimethyl-	213	C14H31N	000112-18-5	72
3		n-Octyl trimethyl ammonium bromide	251	C11H26BrN	002083-68-3	72
4		Dimethyl palmitamine	269	C18H39N	000112-69-6	64
5		1-Undecanamine, N,N-dimethyl-	199	C13H29N	017373-28-3	56



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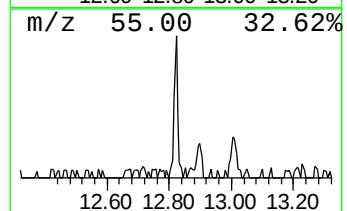
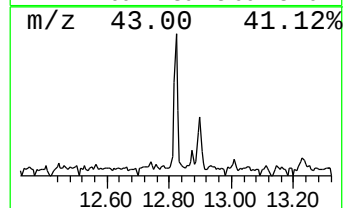
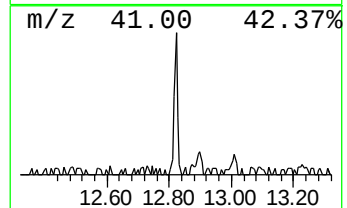
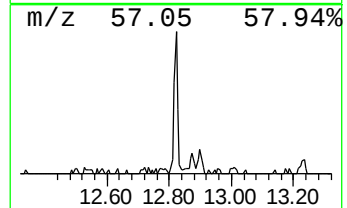
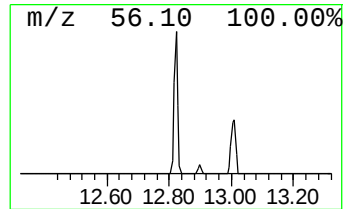
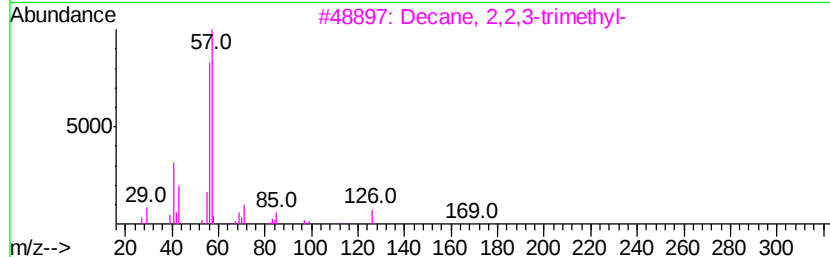
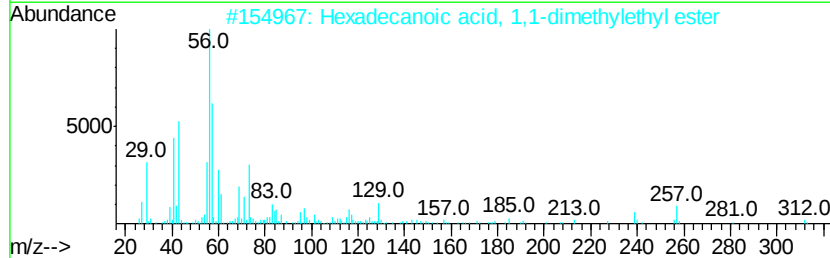
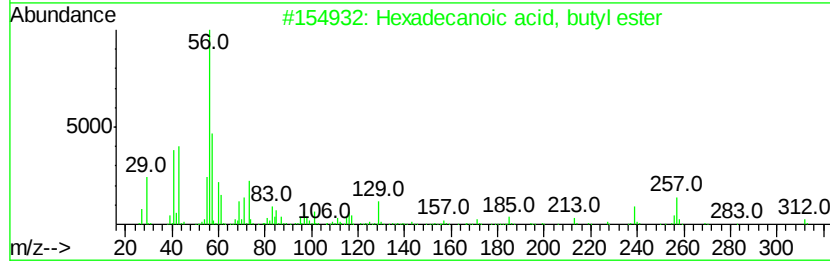
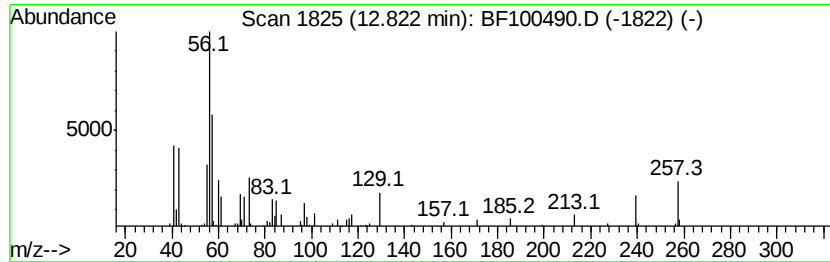
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.82	2.31 ng	87812	Chrysene-d12	14.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	80
3		Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	35
4		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5		Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.20	2.7	ng	109584	1	6.90	822855	20.0
2-Pentanone, 4-hy...	5.12	6.9	ng	282826	1	6.90	822855	20.0
unknown6.67	6.67	54.6	ng	2246900	1	6.90	822855	20.0
Dodecyltrimethyla...	9.89	6.0	ng	322221	3	9.94	1069720	20.0
Hexadecanoic acid...	12.82	2.3	ng	87812	5	14.06	761204	20.0