

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100417\
 Data File : BF099079.D
 Acq On : 4 Oct 2017 21:00
 Operator : SJ/JU
 Sample : I5616-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 STONE-SP-A-COMP

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-BF092317.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	2.169	10	14	21	rVB	149915	199845	5.57%	0.654%
2	2.999	149	155	162	rVB	45853	72408	2.02%	0.237%
3	5.098	507	512	526	rVB	549393	778215	21.69%	2.547%
4	5.493	573	579	582	rBV	3004337	3157733	88.02%	10.333%
5	6.498	744	750	753	rBV	2826243	3173072	88.45%	10.384%
6	6.640	768	774	777	rBV	2959158	3205673	89.36%	10.490%
7	6.863	808	812	816	rBV	973627	775197	21.61%	2.537%
8	7.022	834	839	842	rBV	2794574	2494958	69.55%	8.165%
9	7.428	903	908	911	rBV	1933239	2023707	56.41%	6.622%
10	8.145	1025	1030	1033	rBV	1280830	1057311	29.47%	3.460%
11	9.222	1207	1213	1216	rBV	3720175	3587327	100.00%	11.739%
12	9.610	1275	1279	1282	rBV	558458	448085	12.49%	1.466%
13	9.898	1323	1328	1332	rBV	1231260	1153316	32.15%	3.774%
14	10.322	1398	1400	1403	rVB	54132	37054	1.03%	0.121%
15	10.692	1455	1463	1466	rBV	2002880	1996024	55.64%	6.532%
16	10.792	1477	1480	1485	rBV	63011	62245	1.74%	0.204%
17	11.386	1577	1581	1585	rBV	1323010	1135942	31.67%	3.717%
18	12.974	1846	1851	1854	rBV	3241702	3235218	90.18%	10.587%
19	13.857	1997	2001	2009	rBV	116712	141571	3.95%	0.463%
20	14.027	2026	2030	2033	rBV	969137	858619	23.93%	2.810%
21	14.486	2102	2108	2114	rBV3	52576	83941	2.34%	0.275%
22	15.121	2212	2216	2220	rBV	44991	54955	1.53%	0.180%
23	15.498	2274	2280	2288	rBV	547260	666606	18.58%	2.181%
24	15.939	2350	2355	2361	rBV2	25036	40254	1.12%	0.132%
25	17.545	2621	2628	2635	rBV9	18799	47493	1.32%	0.155%
26	18.362	2759	2767	2776	rBV7	24020	71640	2.00%	0.234%

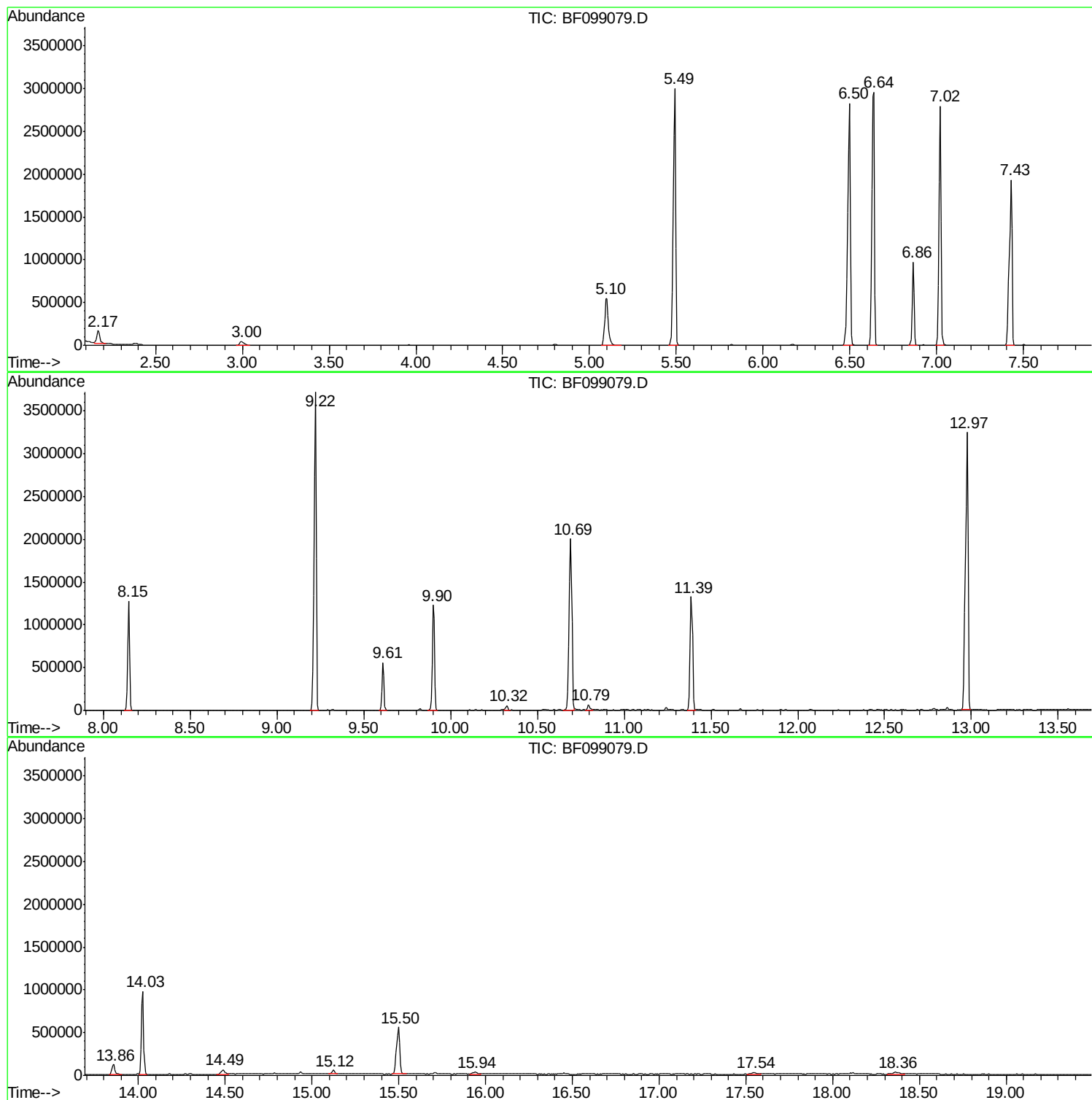
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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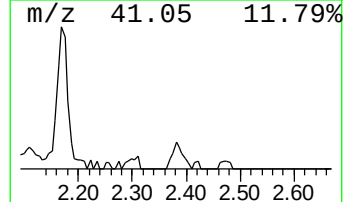
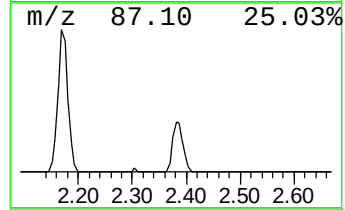
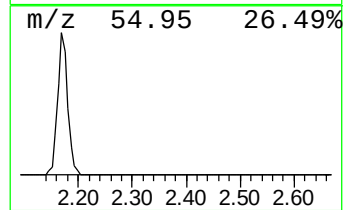
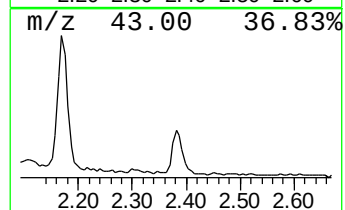
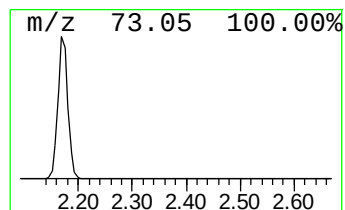
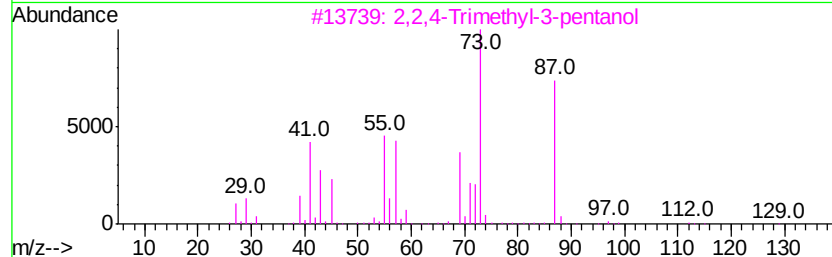
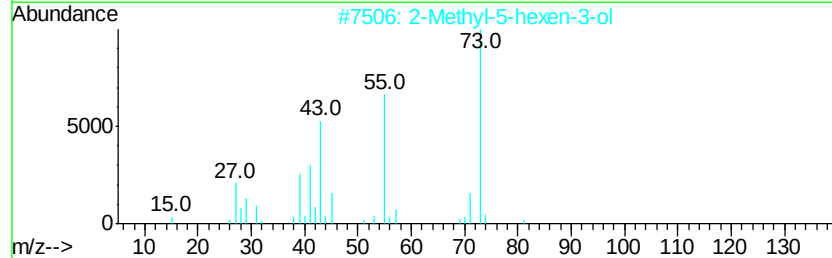
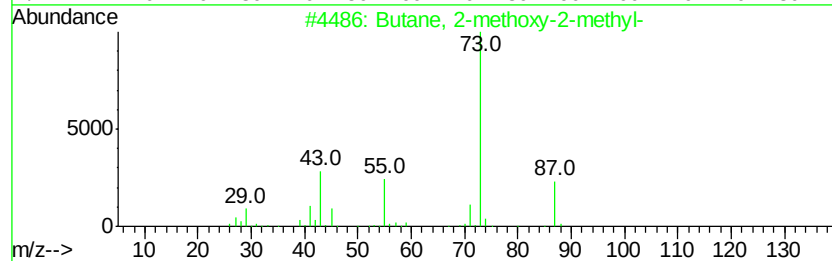
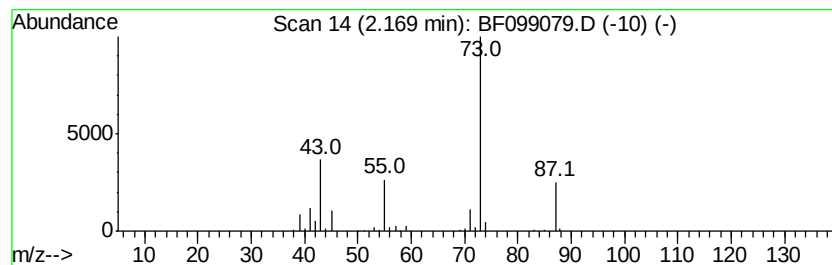
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	5.16 ng	199845	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	40
3		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
5		1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	25



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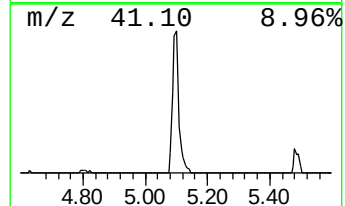
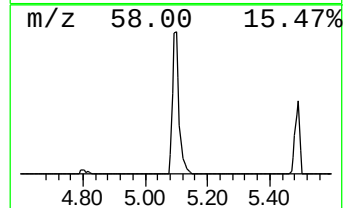
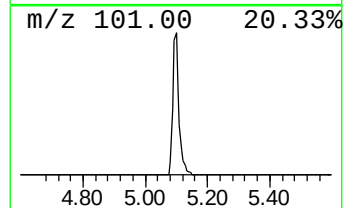
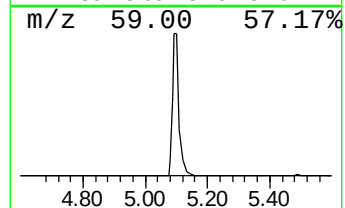
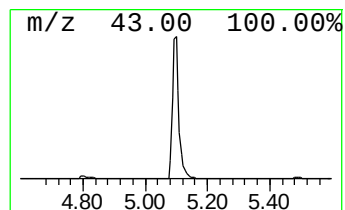
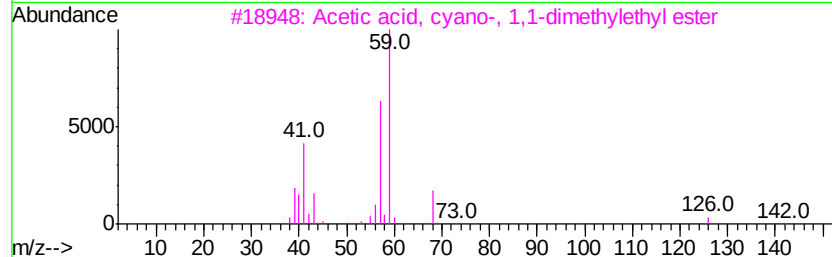
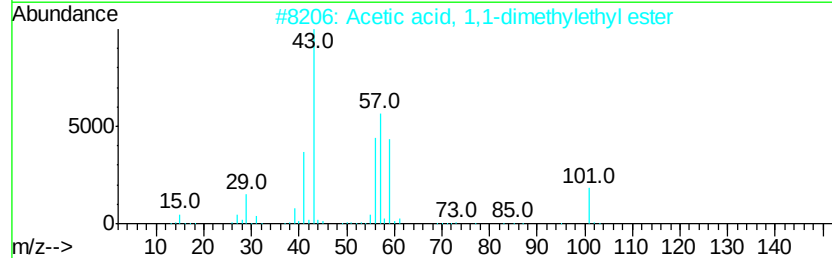
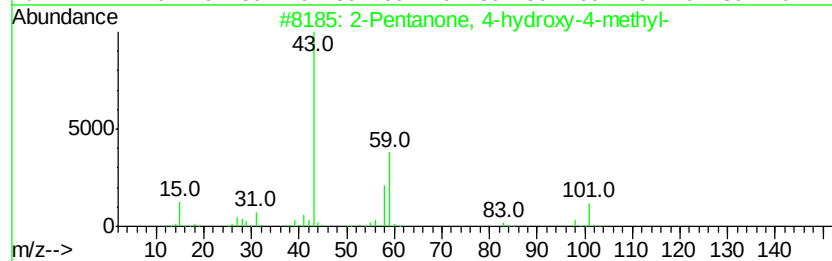
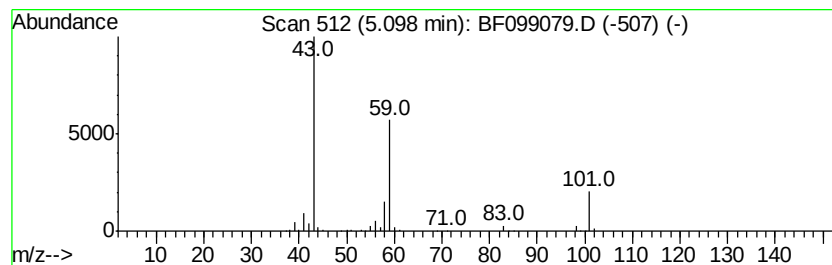
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	20.08 ng	778215	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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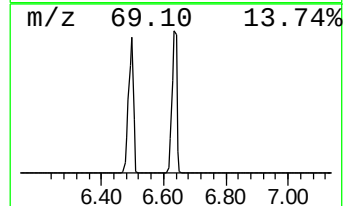
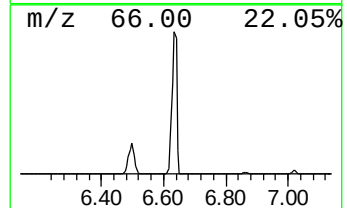
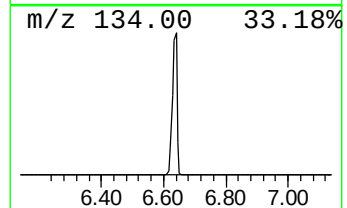
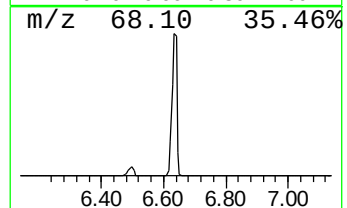
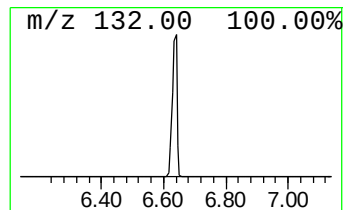
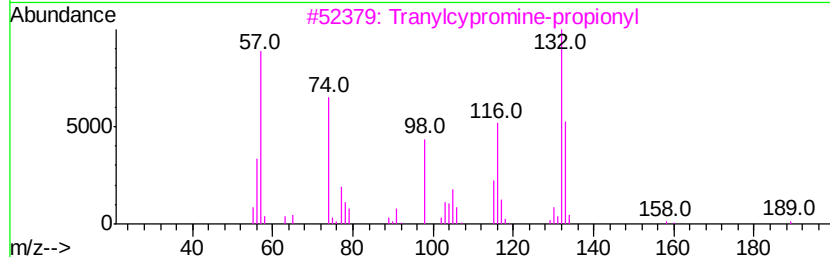
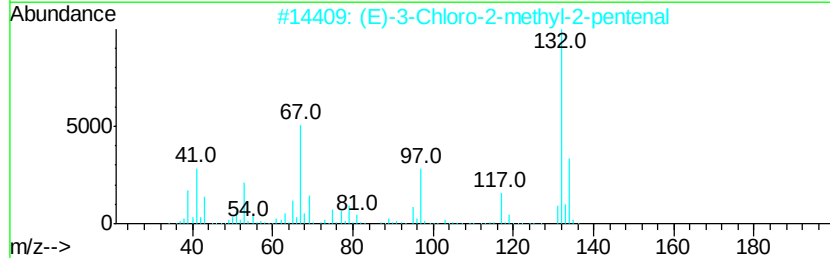
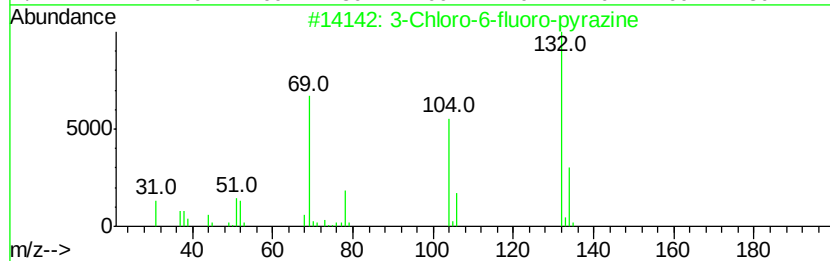
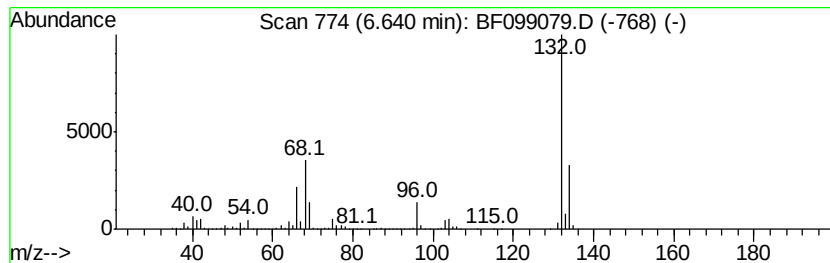
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Peak Number 3 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	82.71 ng	3205670	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	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10



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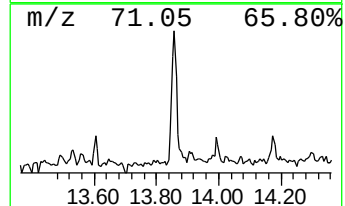
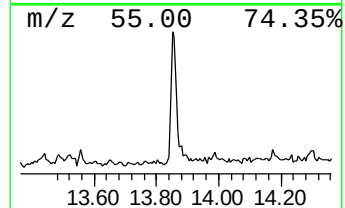
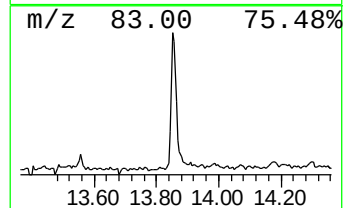
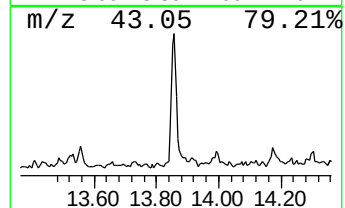
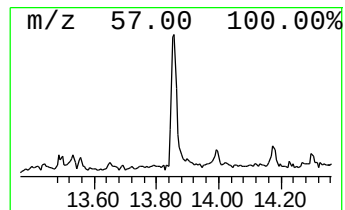
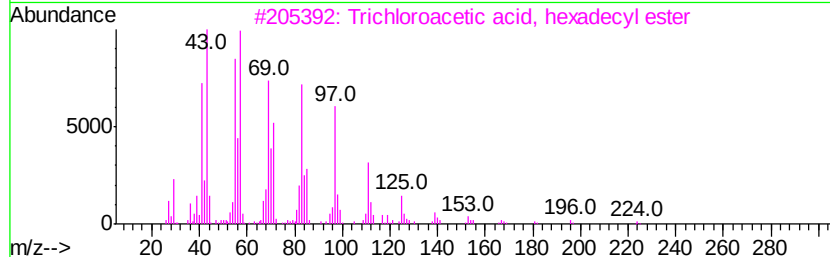
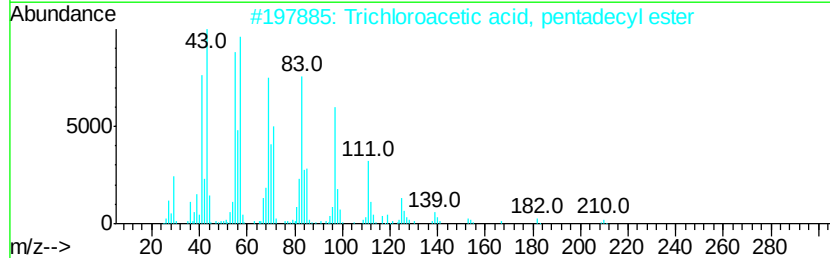
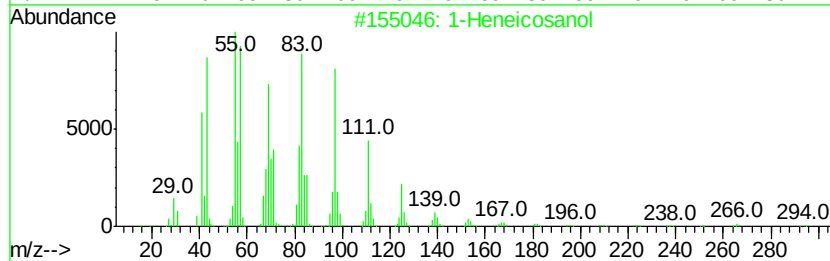
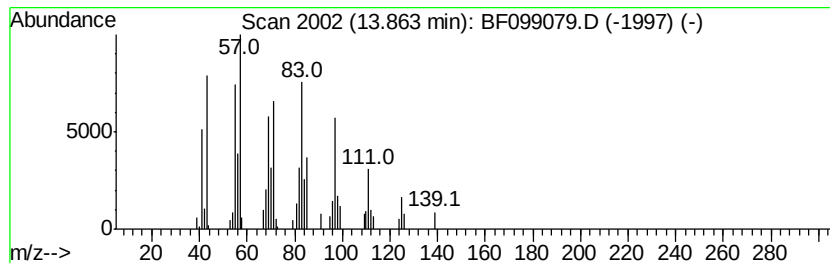
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.86	3.30 ng	141571	Chrysene-d12	14.03	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5	Behenic alcohol	326	C22H46O	000661-19-8	91



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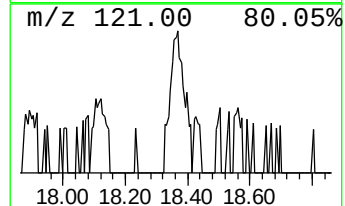
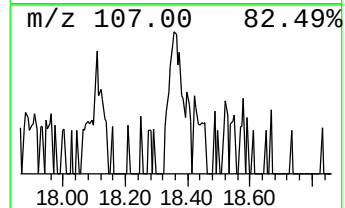
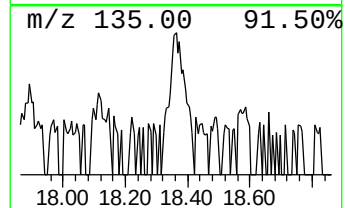
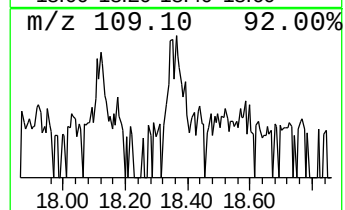
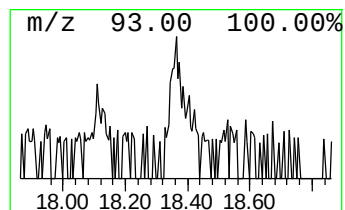
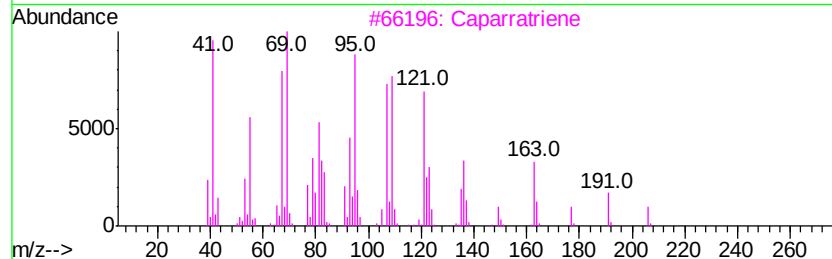
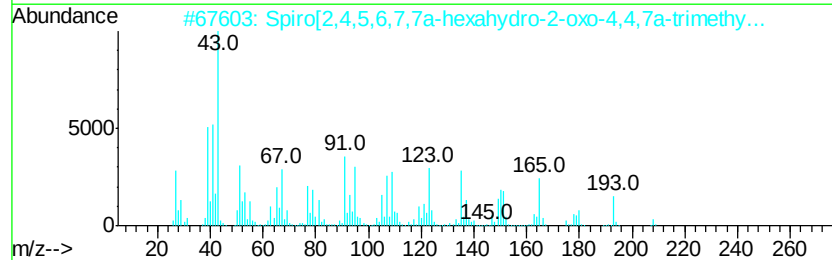
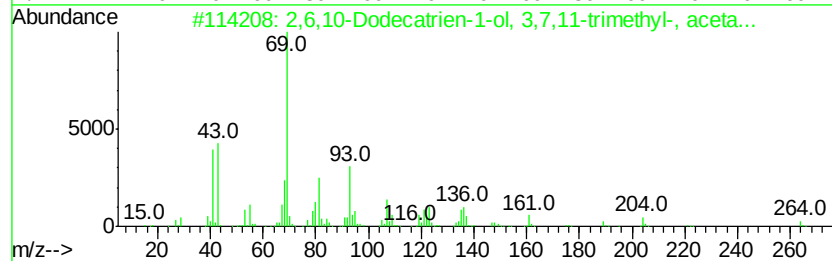
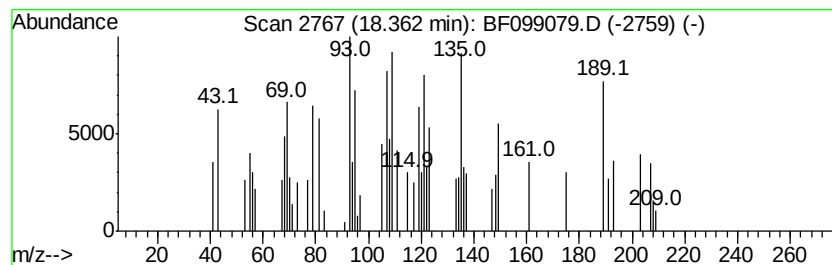
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown18.36 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	2.15 ng	71640	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	38
2		Spiro[2.4,5,6,7,7a-hexahydro-2-o...	208	C12H16O3	1000197-10-9	38
3		Caparratriene	206	C15H26	1000374-08-7	35
4		Ledol	222	C15H26O	000577-27-5	27
5		2,6,10,10-Tetramethylbicyclo[7.2...	204	C15H24	136296-37-2	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.17	5.2	ng	199845	1	6.86	775197	20.0
2-Pentanone, 4-hy...	5.10	20.1	ng	778215	1	6.86	775197	20.0
unknown6.64	6.64	82.7	ng	3205670	1	6.86	775197	20.0
1-Heneicosanol	13.86	3.3	ng	141571	5	14.03	858619	20.0
unknown18.36	18.36	2.1	ng	71640	6	15.50	666606	20.0