

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120916\
 Data File : BF091543.D
 Acq On : 9 Dec 2016 22:38
 Operator : UM/SJ
 Sample : H5917-02
 Misc :
 ALS Vial : 18 Sample Multiplier: 2

Instrument :
 BNA_F
 ClientSampleId :
 URSMW-08

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-BF120916.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	4.978	251	253	256	rBV	764159	1044722	11.33%	1.411%
2	5.413	289	291	294	rBV	3672972	3861773	41.88%	5.215%
3	6.453	379	382	384	rBV	3102115	2910493	31.56%	3.930%
4	6.579	391	393	396	rBV	5381653	6909820	74.94%	9.330%
5	6.807	411	413	416	rBV	2370110	2902681	31.48%	3.919%
6	6.967	424	427	430	rBV	5785720	5838291	63.32%	7.883%
7	7.379	460	463	465	rBV	5077900	5288779	57.36%	7.141%
8	8.099	523	526	528	rBV	4497143	4019760	43.59%	5.428%
9	9.173	617	620	623	rBV	6682814	9220711	100.00%	12.451%
10	9.847	677	679	682	rVB	4164827	4031785	43.73%	5.444%
11	10.636	745	748	751	rBV2	4671251	5598665	60.72%	7.560%
12	10.762	757	759	763	rVB	94619	106581	1.16%	0.144%
13	10.899	766	771	775	rBV2	29199	109148	1.18%	0.147%
14	11.333	806	809	811	rBV	4246889	4126790	44.76%	5.572%
15	11.871	853	856	858	rBV	413495	497320	5.39%	0.672%
16	12.556	914	916	922	rBV5	36837	145335	1.58%	0.196%
17	12.659	922	925	931	rBV	467713	832296	9.03%	1.124%
18	12.922	945	948	950	rBV	7693831	8368072	90.75%	11.299%
19	13.814	1024	1026	1029	rBV2	82900	100515	1.09%	0.136%
20	13.962	1036	1039	1041	rBV	3350434	3265656	35.42%	4.410%
21	14.819	1103	1114	1129	rBV3	254646	2085659	22.62%	2.816%
22	15.379	1159	1163	1166	rBV	2186239	2793406	30.29%	3.772%

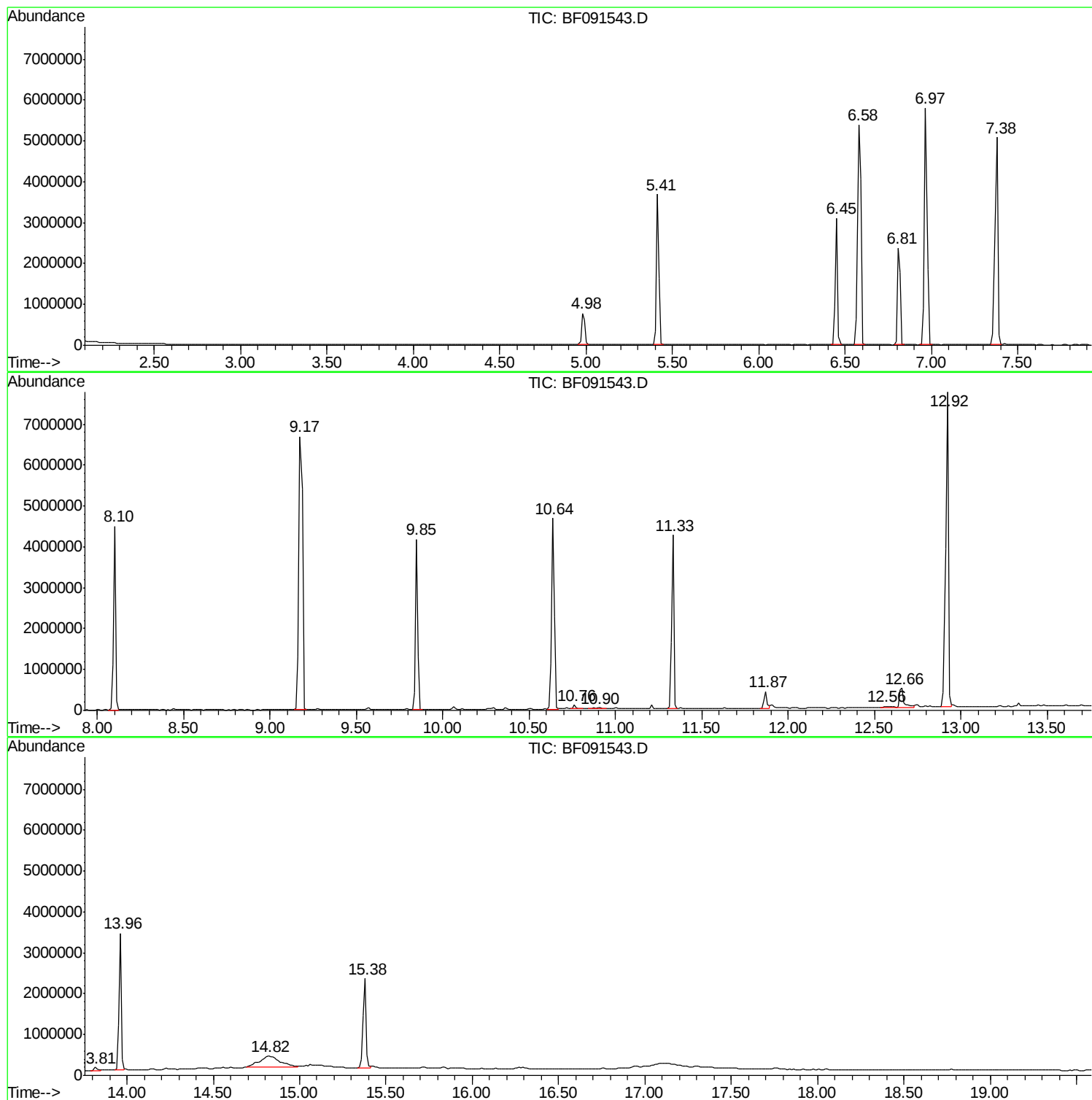
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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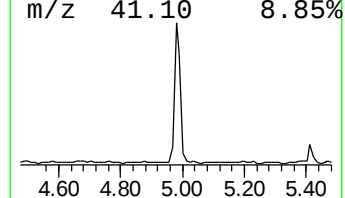
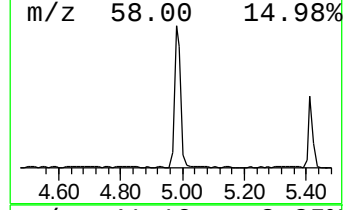
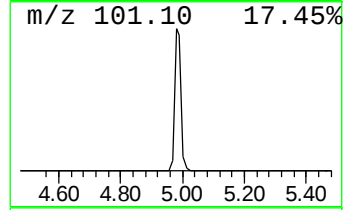
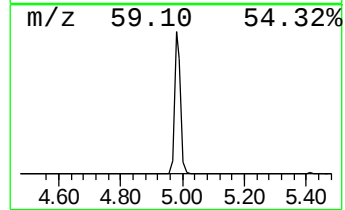
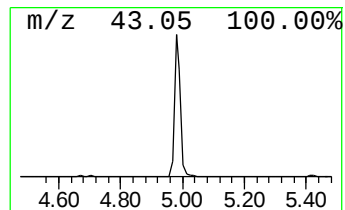
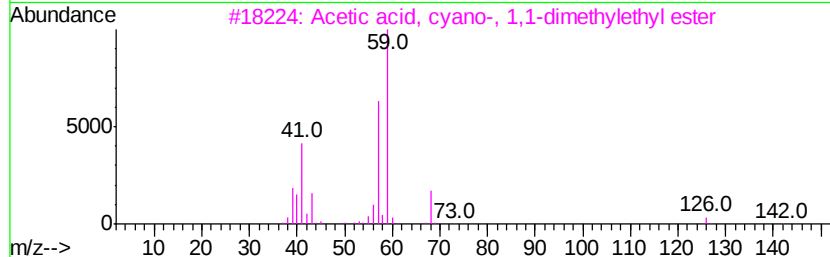
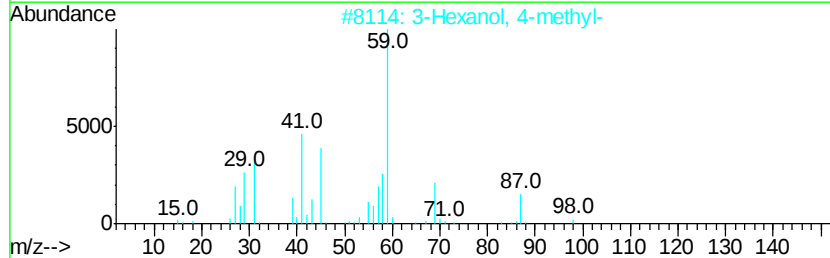
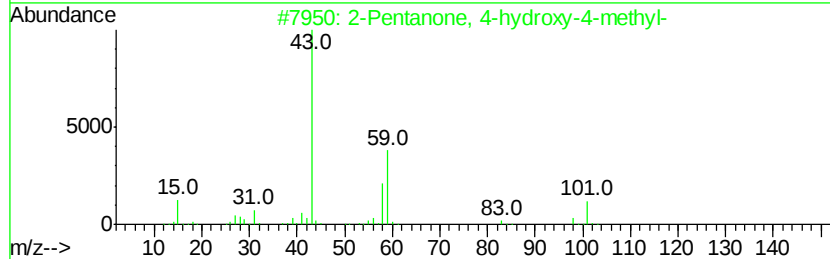
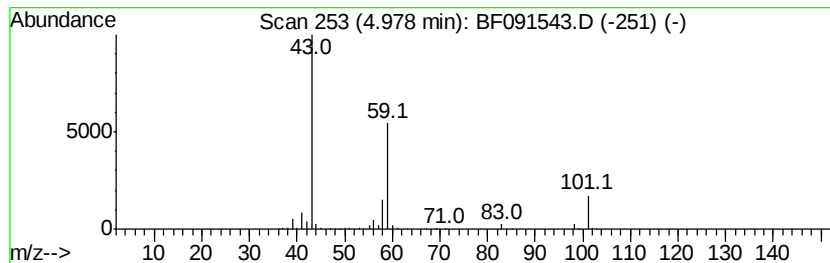
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	7.20 ng	1044720	1,4-Dichlorobenzene-d4	6.81

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	32
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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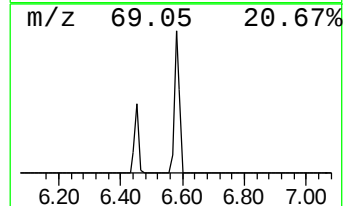
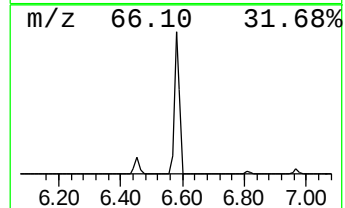
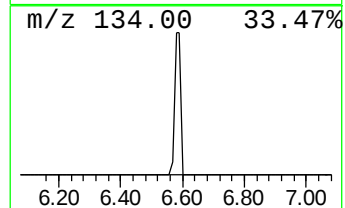
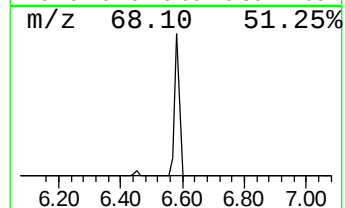
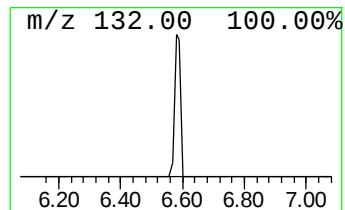
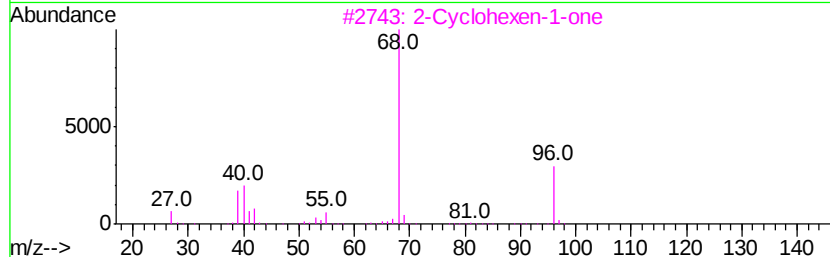
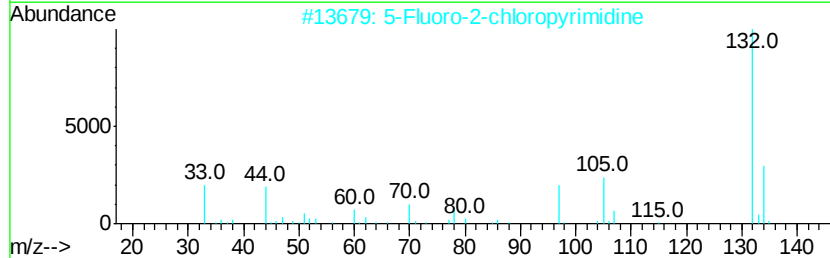
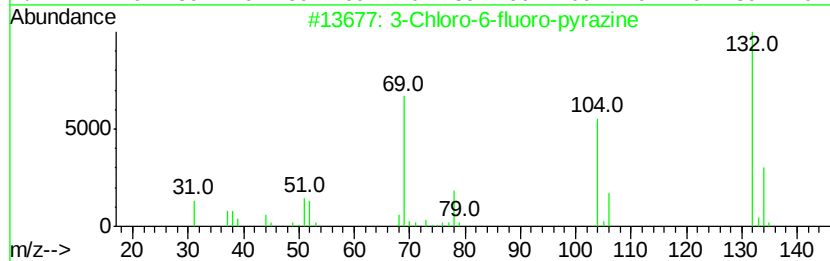
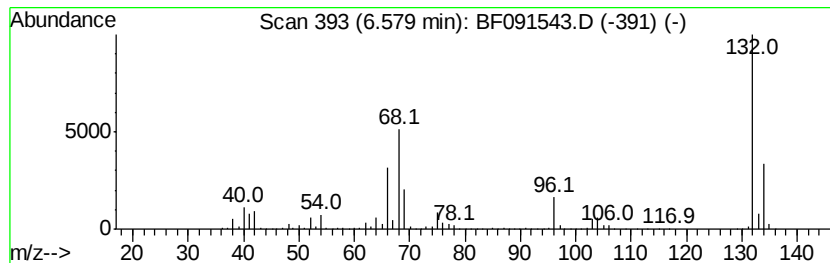
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	47.61 ng	6909820	1,4-Dichlorobenzene-d4	6.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16		
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12		
3	2-Cvclohexen-1-one	96	C6H8O	000930-68-7	10		
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10		
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9		



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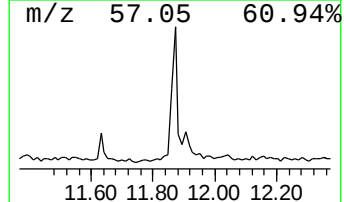
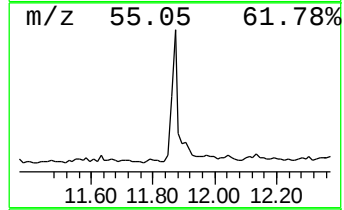
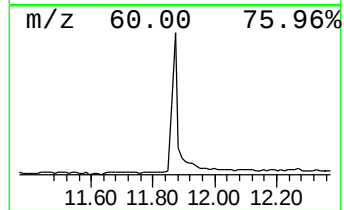
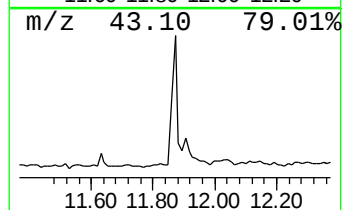
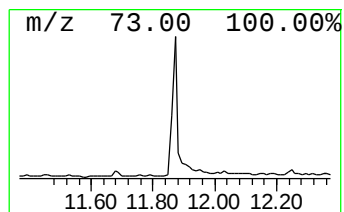
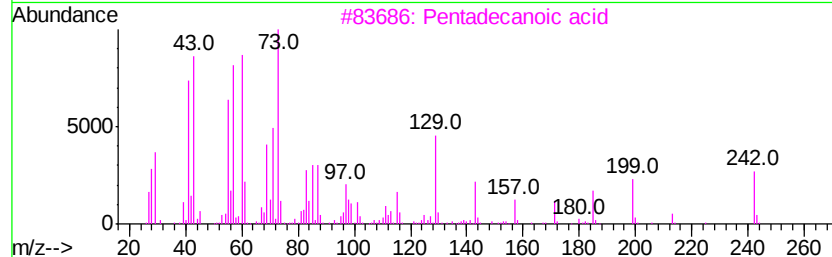
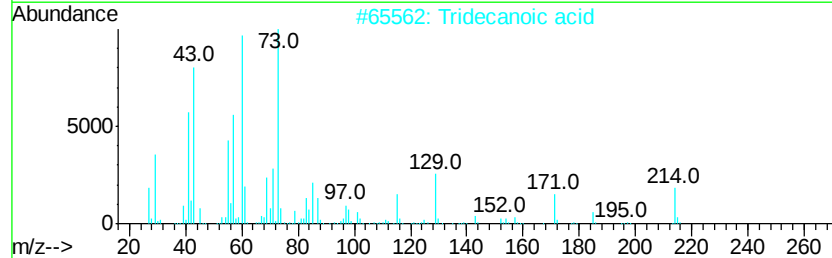
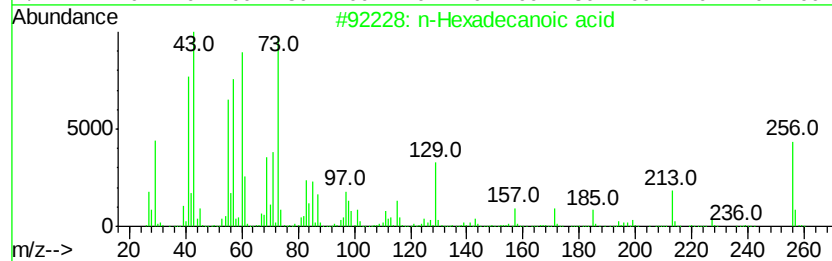
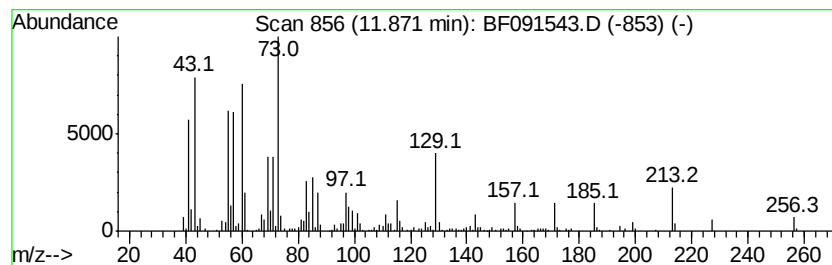
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.87	2.41 ng	497320	Phenanthrene-d10		11.33
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	38



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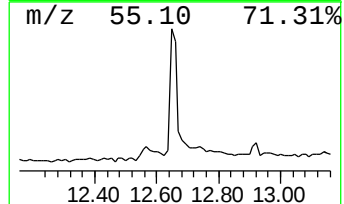
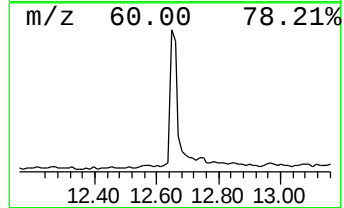
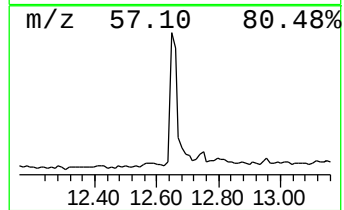
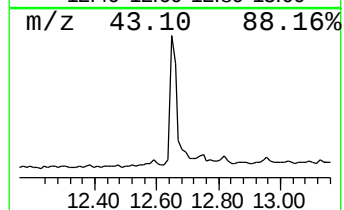
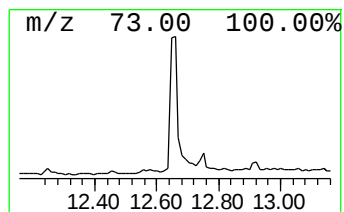
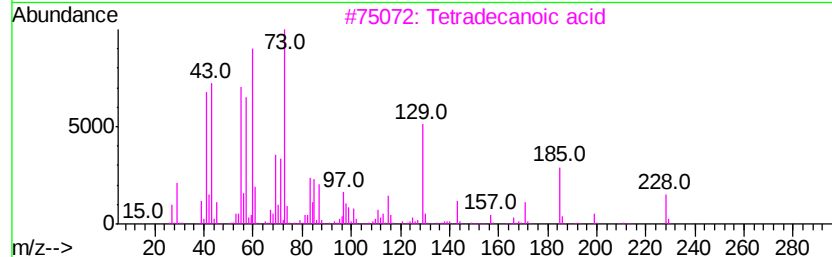
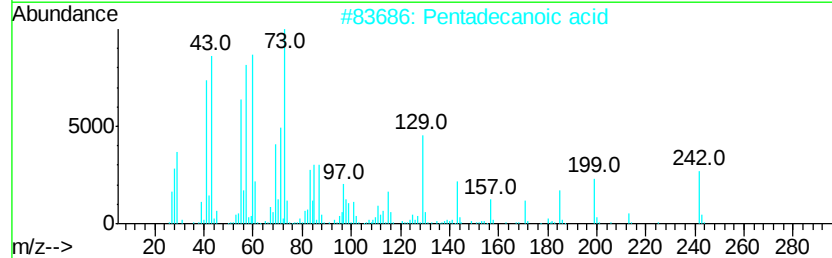
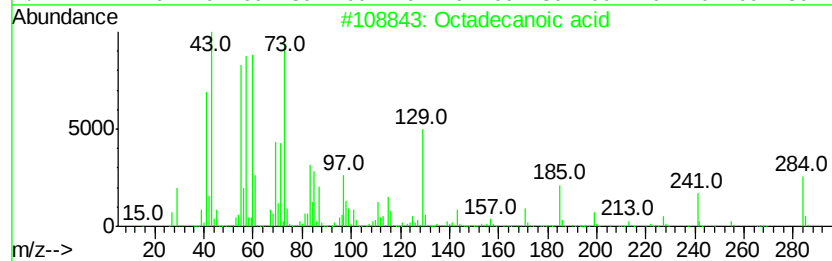
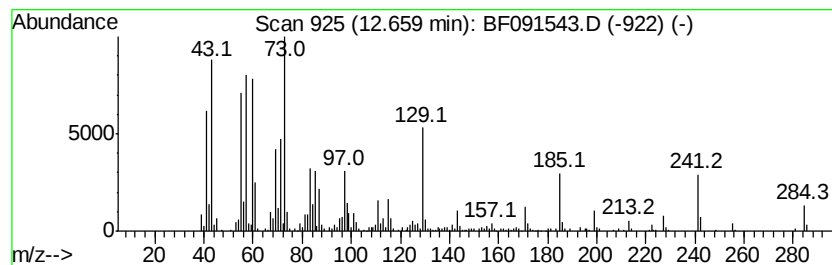
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.66	5.10 ng	832296	Chrysene-d12		13.96
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Tridecanoic acid	214	C13H26O2	000638-53-9	68



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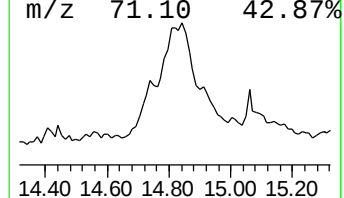
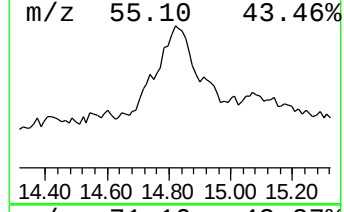
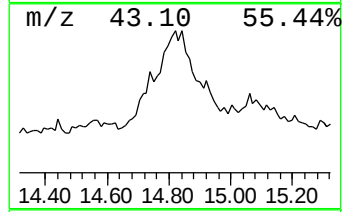
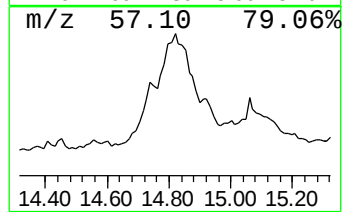
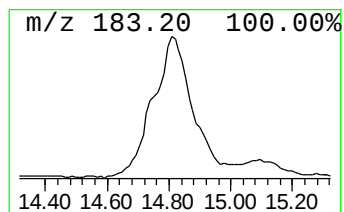
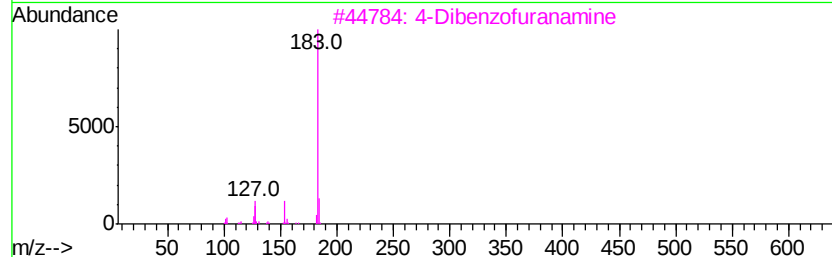
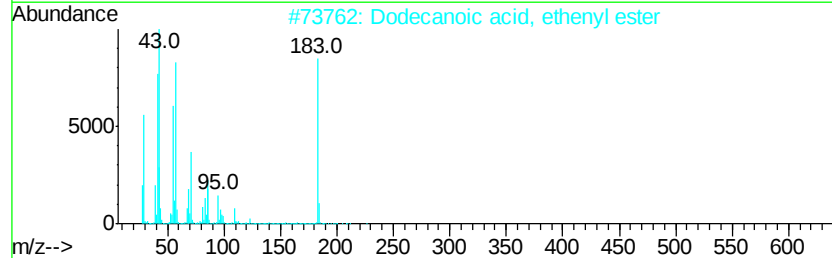
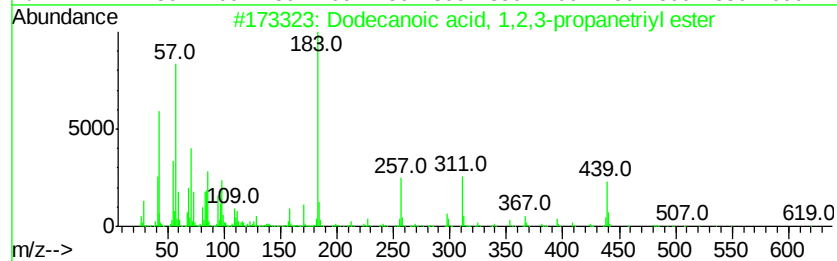
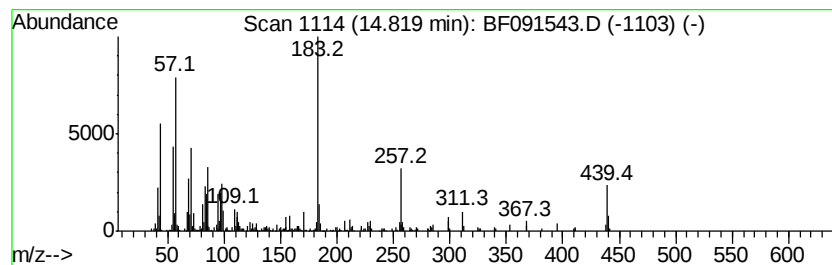
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Dodecanoic acid, 1,2,3-prop... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	14.93 ng	2085660	Perylene-d12	15.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecanoic acid, 1,2,3-propanetr...	639	C39H74O6	000538-24-9	93
2		Dodecanoic acid, ethenyl ester	226	C14H26O2	002146-71-6	50
3		4-Dibenzofuranamine	183	C12H9NO	050548-43-1	47
4		3-Dibenzofuranamine	183	C12H9NO	004106-66-5	38
5		4-Nitrophenyl laurate	321	C18H27NO4	001956-11-2	35



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.98	7.2	ng	1044720	1	6.81	2902680	20.0
unknown6.58	6.58	47.6	ng	6909820	1	6.81	2902680	20.0
n-Hexadecanoic acid	11.87	2.4	ng	497320	4	11.33	4126790	20.0
Octadecanoic acid	12.66	5.1	ng	832296	5	13.96	3265660	20.0
Dodecanoic acid, ...	14.82	14.9	ng	2085660	6	15.38	2793410	20.0