

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121416\
 Data File : BF091588.D
 Acq On : 14 Dec 2016 17:06
 Operator : UM/SJ
 Sample : H5986-02
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 000105-1F-038

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	4.956	248	251	255	rBV	670384	890835	10.15%	1.522%
2	5.390	286	289	291	rBV	4020728	3790194	43.20%	6.474%
3	6.430	377	380	382	rBV	2840679	2751566	31.36%	4.700%
4	6.556	389	391	394	rBV	4973024	5955269	67.88%	10.172%
5	6.796	409	412	414	rBV	1313056	1638580	18.68%	2.799%
6	6.945	423	425	428	rVB	4833774	5551907	63.28%	9.483%
7	7.356	458	461	464	rBV	4500772	4545441	51.81%	7.764%
8	8.076	522	524	527	rBV	2668352	2290281	26.11%	3.912%
9	9.162	616	619	620	rBV	8209607	8773318	100.00%	14.986%
10	9.482	642	647	648	rBV5	95372	181164	2.06%	0.309%
11	9.551	652	653	655	rVB	231126	172080	1.96%	0.294%
12	9.688	663	665	667	rBV	85284	117653	1.34%	0.201%
13	9.756	667	671	675	rVV5	84811	263442	3.00%	0.450%
14	9.825	675	677	679	rVV	1823813	2313046	26.36%	3.951%
15	9.893	679	683	686	rBV6	60052	150034	1.71%	0.256%
16	10.122	701	703	705	rVV3	139981	178686	2.04%	0.305%
17	10.625	744	747	749	rBV	3392854	4790379	54.60%	8.183%
18	11.311	805	807	809	rBV	2511796	2255709	25.71%	3.853%
19	11.871	854	856	860	rVB	1084114	1059761	12.08%	1.810%
20	12.648	922	924	927	rBV	1014463	1045320	11.91%	1.786%
21	12.899	943	946	949	rVB	5390851	6453369	73.56%	11.023%
22	13.802	1023	1025	1030	rVB3	163452	243278	2.77%	0.416%
23	13.940	1035	1037	1040	rBV	1324883	1643071	18.73%	2.807%
24	15.357	1158	1161	1163	rBV	1219655	1488459	16.97%	2.543%

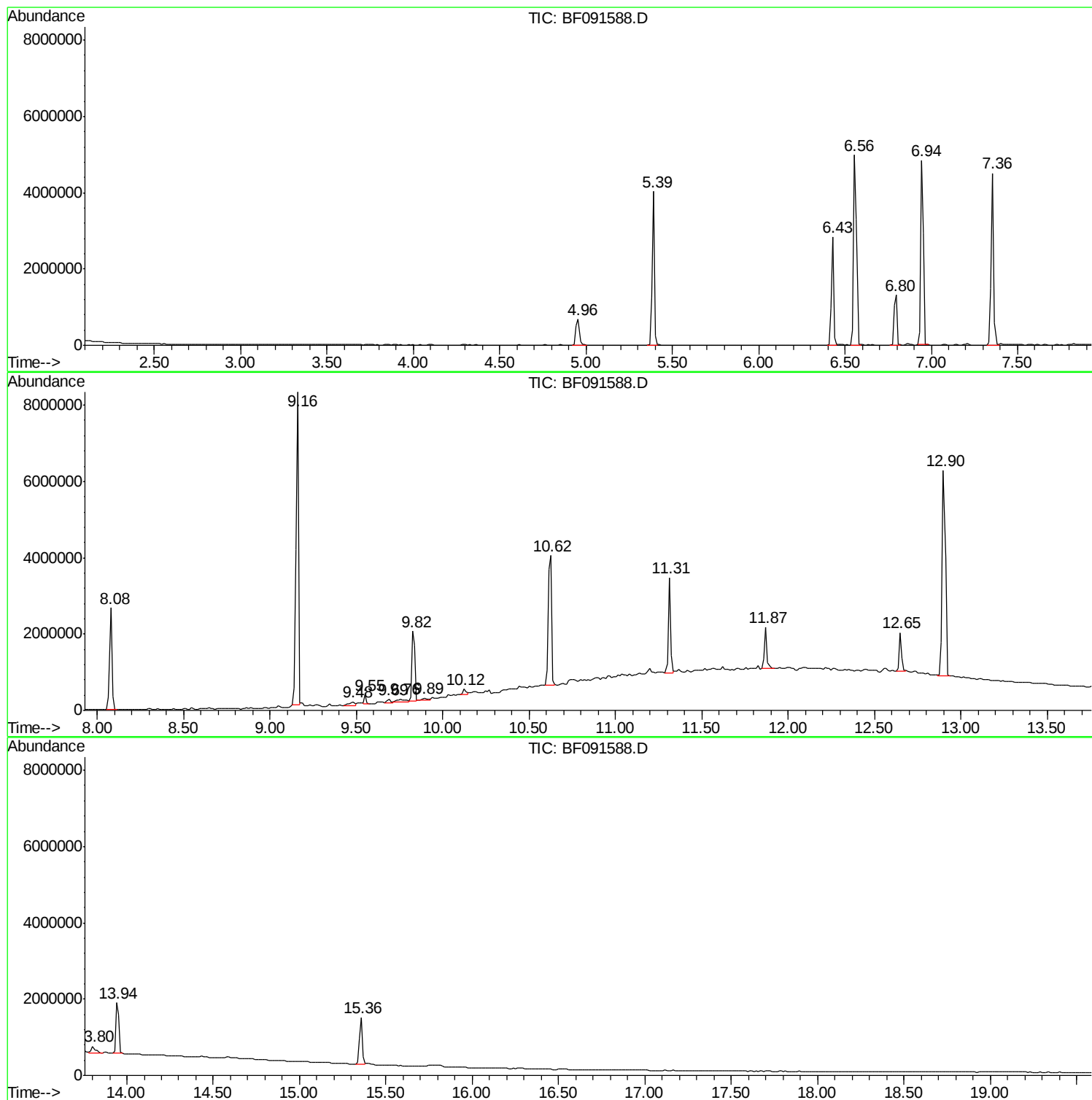
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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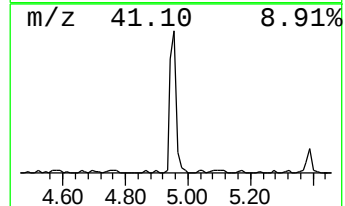
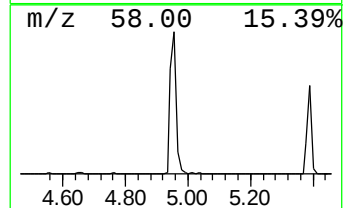
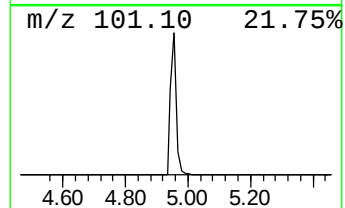
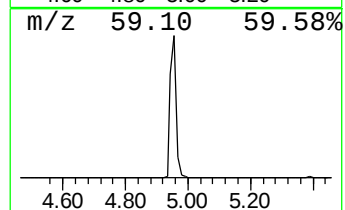
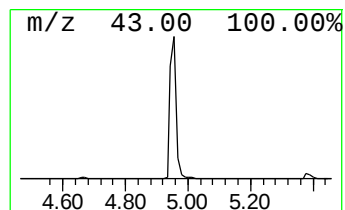
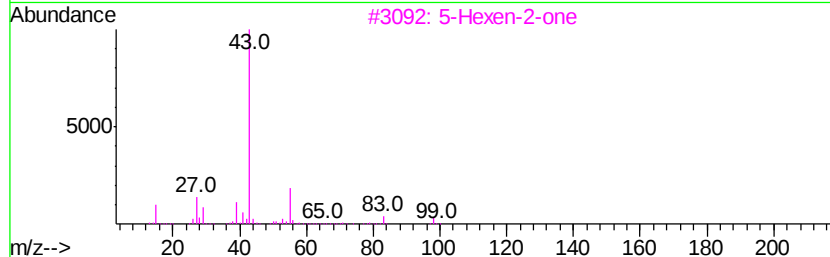
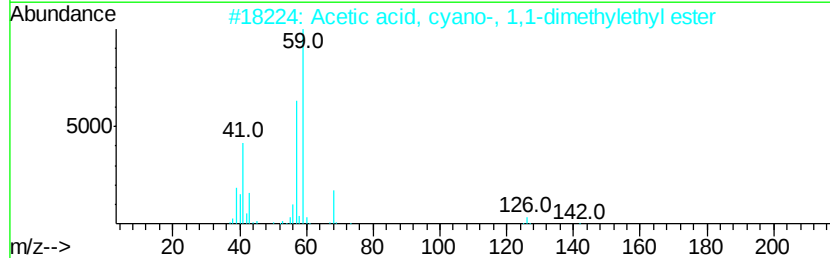
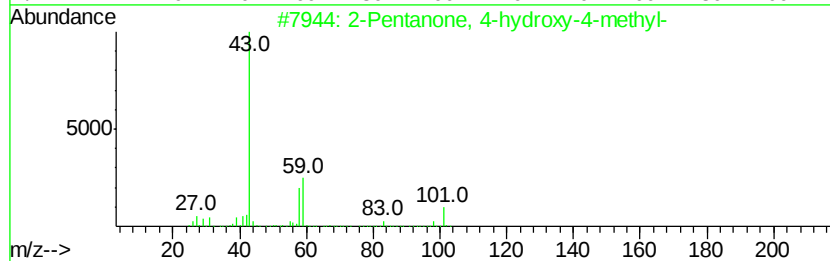
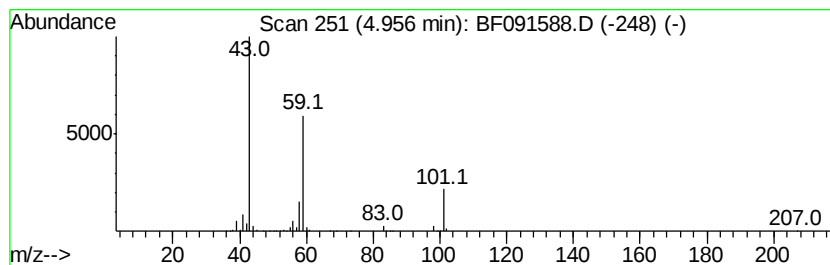
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	10.87 ng	890835	1,4-Dichlorobenzene-d4	6.80

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, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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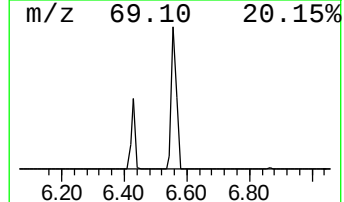
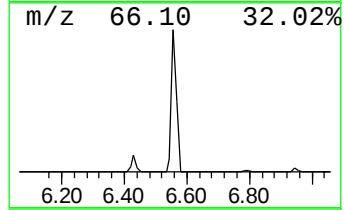
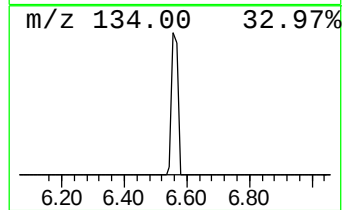
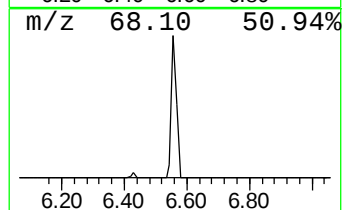
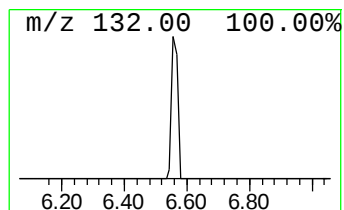
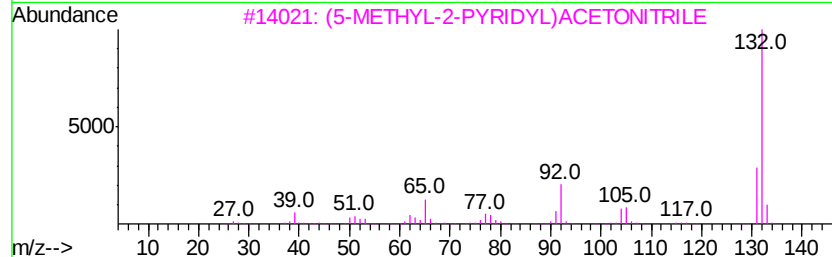
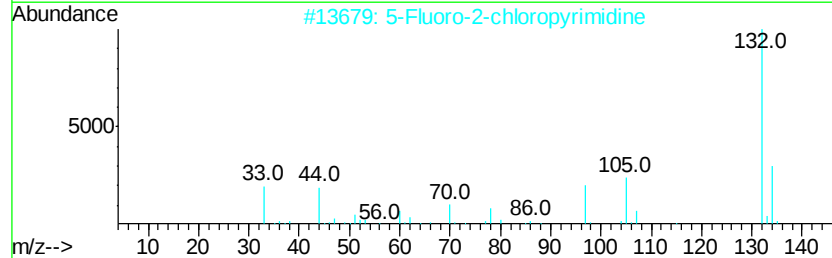
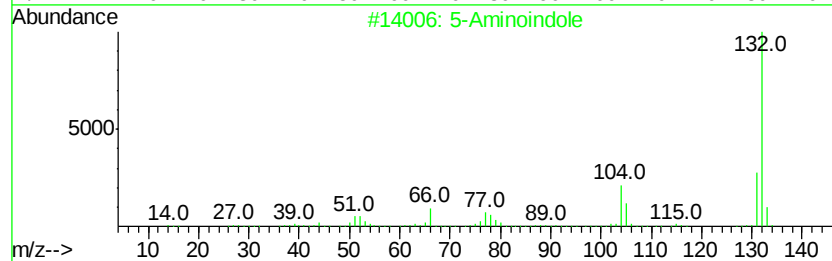
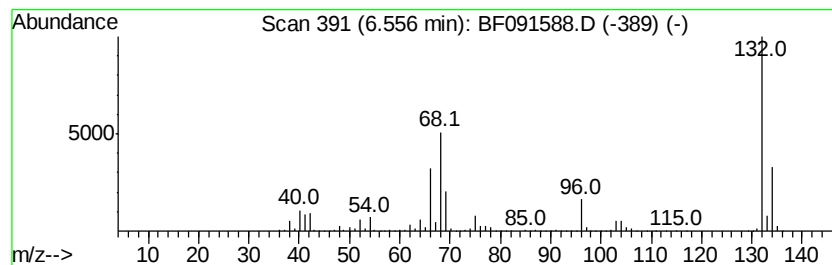
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	72.69 ng	5955270	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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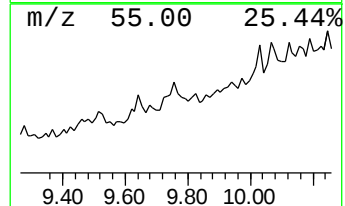
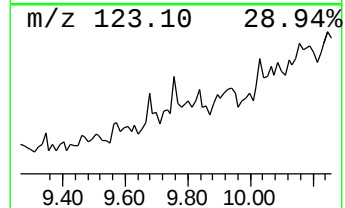
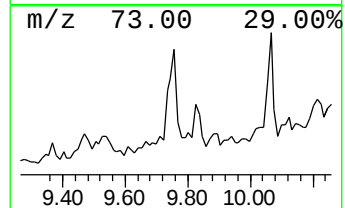
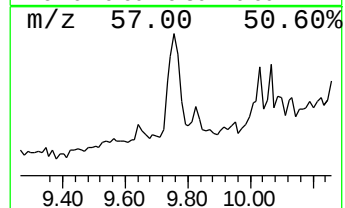
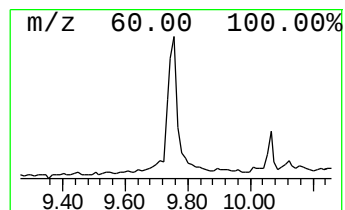
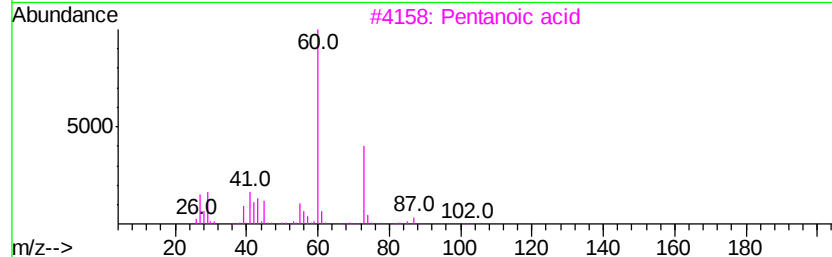
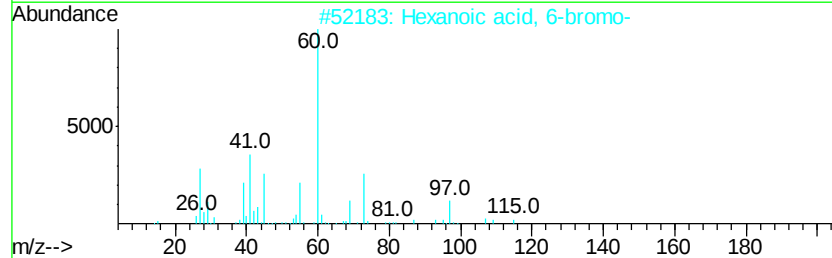
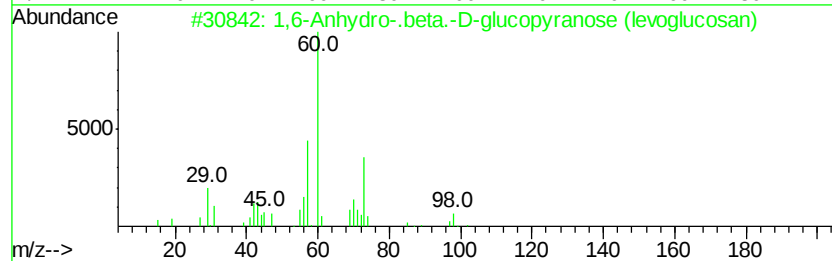
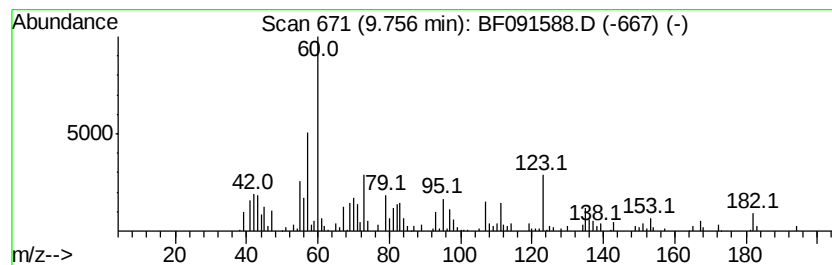
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Peak Number 4 unknown9.76 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.76	2.28 ng	263442	Acenaphthene-d10	9.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	47
2		Hexanoic acid, 6-bromo-	194	C6H11BrO2	004224-70-8	47
3		Pentanoic acid	102	C5H10O2	000109-52-4	46
4		Chloro-methyl-methoxy-amine	95	C2H6ClNO	070569-68-5	43
5		.beta.-D-Ribopyranoside, methyl	164	C6H12O5	017289-61-1	43



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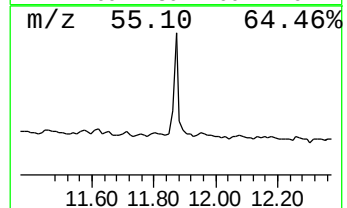
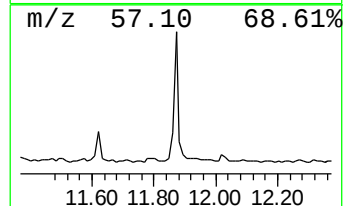
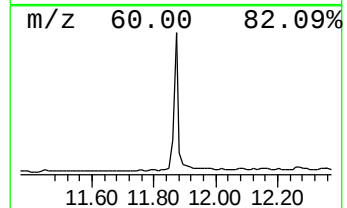
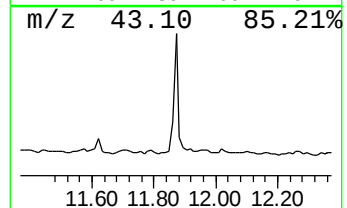
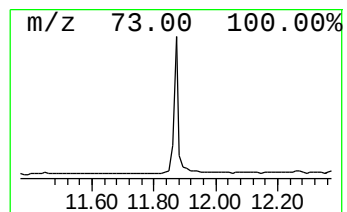
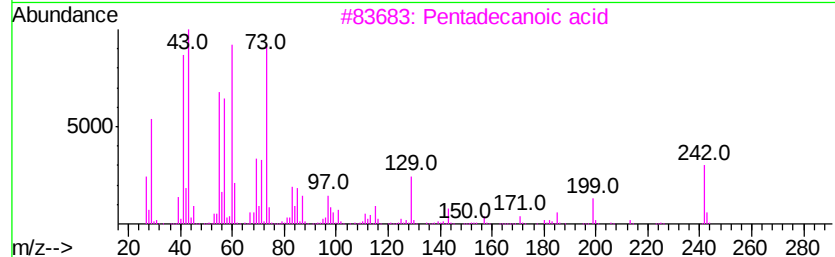
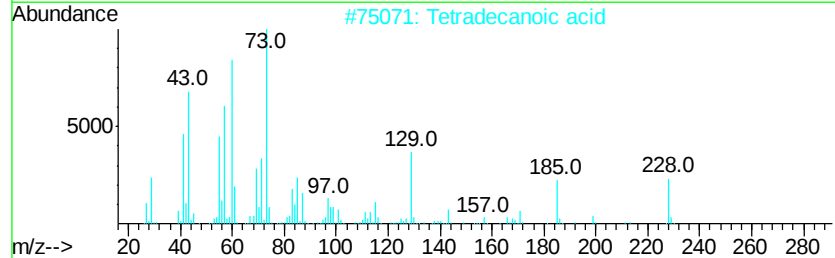
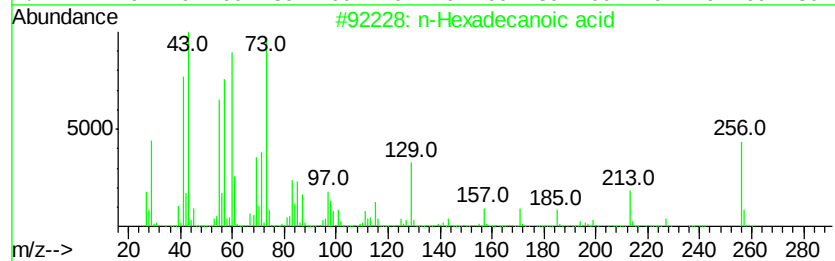
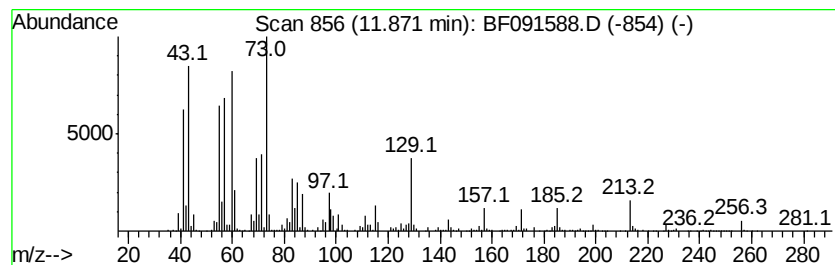
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.87	9.40 ng	1059760	Phenanthrene-d10	11.31	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
4	Tridecanoic acid	214	C13H26O2	000638-53-9	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68



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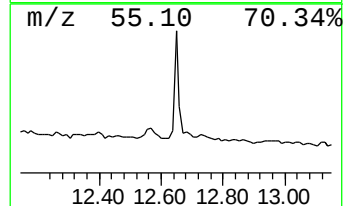
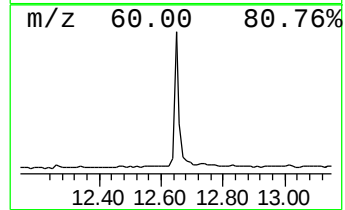
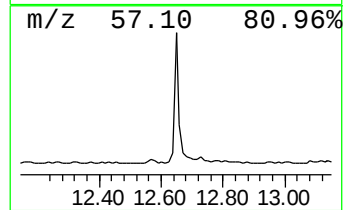
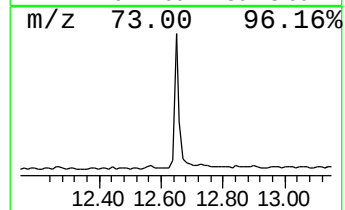
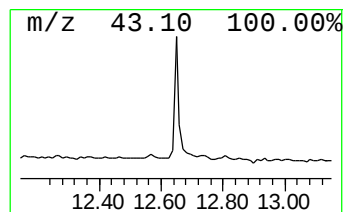
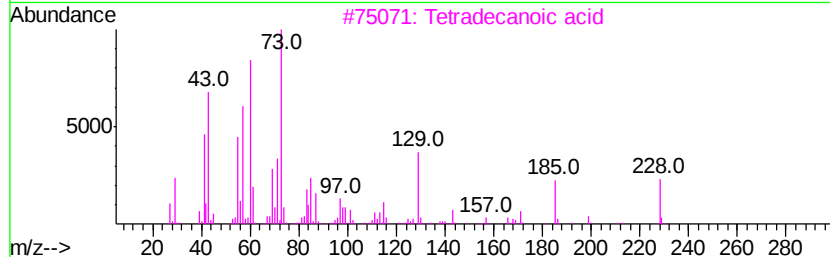
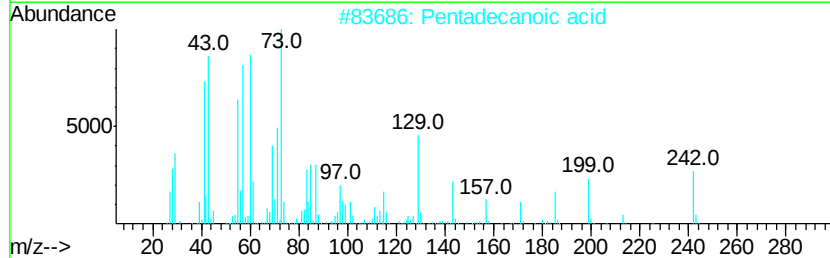
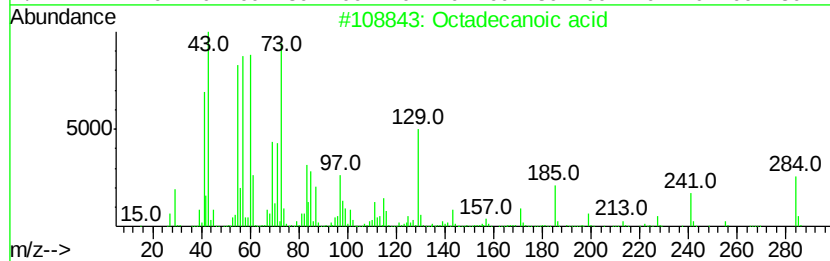
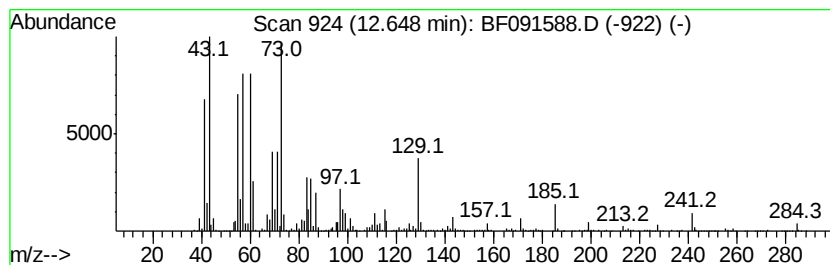
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Peak Number 6 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.65	12.72 ng	1045320	Chrysene-d12	13.94	
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	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	86
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76



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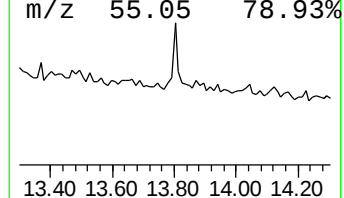
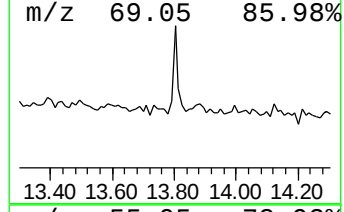
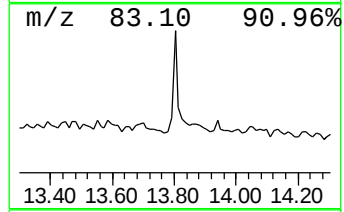
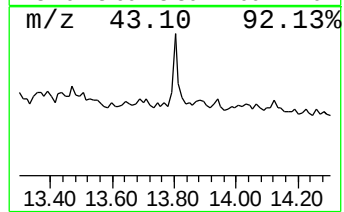
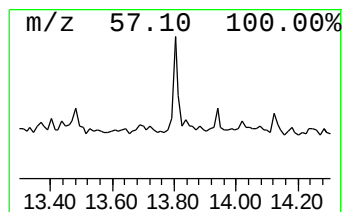
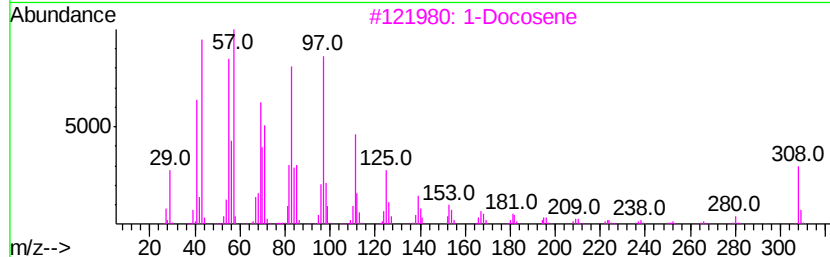
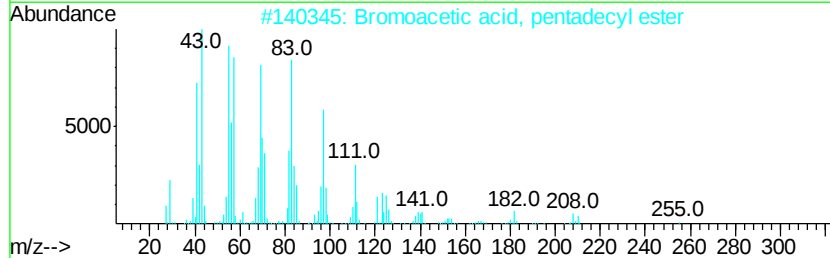
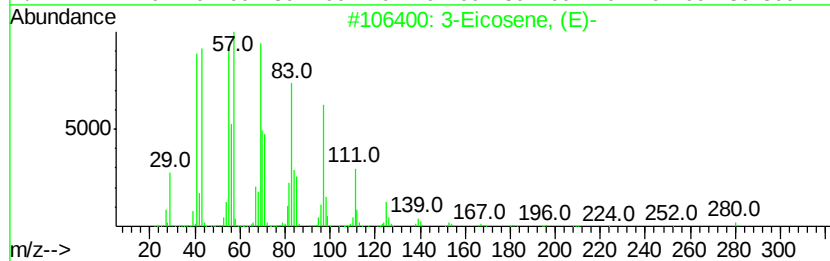
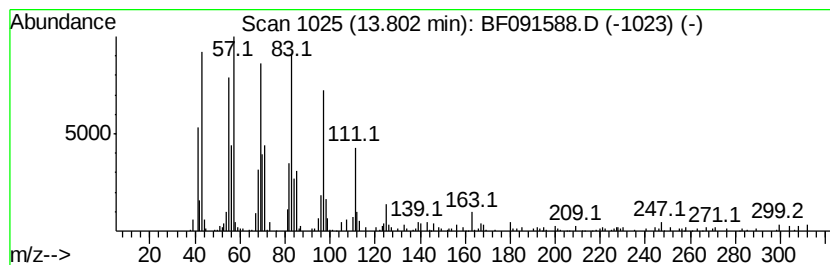
Instrument :
BNA_F
ClientSampleId :
000105-1F-038

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 7 3-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.80	2.96 ng	243278	Chrysene-d12	13.94		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3	Eicosene, (E)-	280	C20H40	074685-33-9	91
2		Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	90
3		1-Docosene	308	C22H44	001599-67-3	90
4		1-Heptadecanol	256	C17H36O	001454-85-9	87
5		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121416\
Data File : BF091588.D
Acq On : 14 Dec 2016 17:06
Operator : UM/SJ
Sample : H5986-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
000105-1F-038

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.96	10.9	ng	890835	1	6.80	1638580	20.0
unknown6.56	6.56	72.7	ng	5955270	1	6.80	1638580	20.0
unknown9.76	9.76	2.3	ng	263442	3	9.82	2313050	20.0
n-Hexadecanoic acid	11.87	9.4	ng	1059760	4	11.31	2255710	20.0
Octadecanoic acid	12.65	12.7	ng	1045320	5	13.94	1643070	20.0
3-Eicosene, (E)-	13.80	3.0	ng	243278	5	13.94	1643070	20.0