

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
 Data File : BF086793.D
 Acq On : 8 May 2016 00:26
 Operator : UM/SJ
 Sample : H2882-05
 Misc :
 ALS Vial : 63 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MWHR4-9

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-BF050416.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	4.876	242	244	248	rBV	126033	199857	3.09%	0.450%
2	5.310	280	282	299	rBV	2664115	3001732	46.45%	6.763%
3	5.710	313	317	322	rBV	40025	65707	1.02%	0.148%
4	6.362	372	374	379	rBV	1959074	1964973	30.41%	4.427%
5	6.476	382	384	387	rBV	4736165	4654622	72.03%	10.488%
6	6.705	402	404	406	rBV	972265	1113980	17.24%	2.510%
7	6.853	415	417	420	rBV	3293671	4219415	65.29%	9.507%
8	7.276	451	454	456	rBV	3585837	3864379	59.80%	8.707%
9	7.447	468	469	475	rVB2	91236	112568	1.74%	0.254%
10	7.928	508	511	514	rBV	151940	148342	2.30%	0.334%
11	7.985	514	516	519	rBV	1271256	1432468	22.17%	3.228%
12	9.070	607	611	613	rBV	5724302	6462419	100.00%	14.561%
13	9.471	643	646	650	rBV	59097	92866	1.44%	0.209%
14	9.676	662	664	665	rBV	95572	83302	1.29%	0.188%
15	9.733	665	669	672	rVV2	1524378	1790120	27.70%	4.033%
16	10.179	705	708	709	rVB	107873	126991	1.97%	0.286%
17	10.259	713	715	718	rBV	51380	67679	1.05%	0.152%
18	10.385	724	726	730	rBV	196497	216590	3.35%	0.488%
19	10.533	736	739	745	rBV2	3077917	4223567	65.36%	9.517%
20	10.648	747	749	755	rVB	436539	462436	7.16%	1.042%
21	10.831	763	765	770	rVB2	96985	154180	2.39%	0.347%
22	11.094	784	788	796	rBV2	49993	69762	1.08%	0.157%
23	11.219	796	799	801	rBV	1408650	1462517	22.63%	3.295%
24	11.756	844	846	854	rBV2	83181	139837	2.16%	0.315%
25	12.545	912	915	920	rBV	42485	84931	1.31%	0.191%
26	12.625	920	922	925	rBV	196785	226084	3.50%	0.509%
27	12.705	925	929	935	rVB2	106757	133756	2.07%	0.301%
28	12.808	935	938	940	rBV	4182027	5245328	81.17%	11.819%
29	13.334	982	984	986	rBV	159431	149861	2.32%	0.338%
30	13.368	986	987	989	rVV	214073	239680	3.71%	0.540%
31	13.711	1014	1017	1023	rBV	81458	141287	2.19%	0.318%
32	13.848	1026	1029	1031	rBV	810793	1055407	16.33%	2.378%
33	14.922	1120	1123	1125	rBV	40739	69201	1.07%	0.156%
34	15.220	1146	1149	1156	rBV	594232	905517	14.01%	2.040%

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Misc :
ALS Vial : 63 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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-BF050416.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

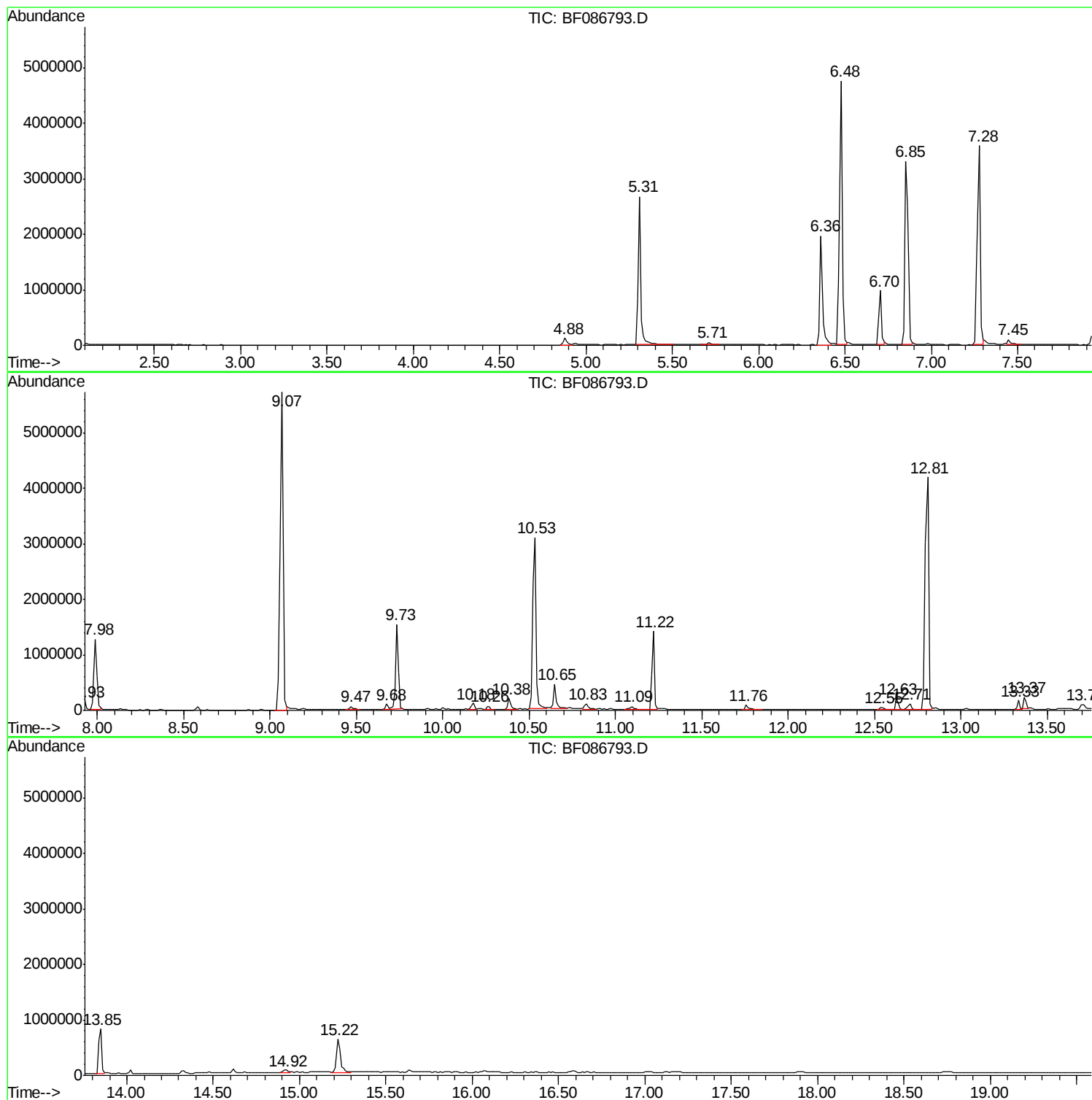
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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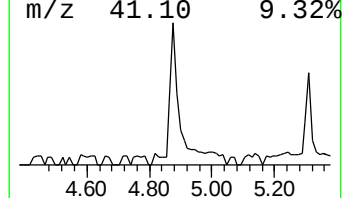
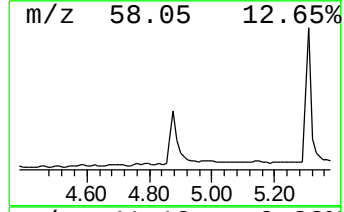
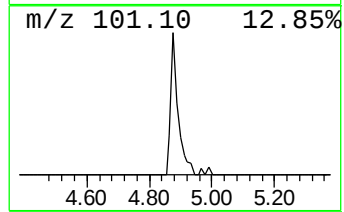
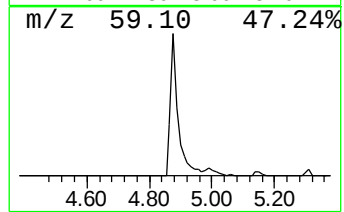
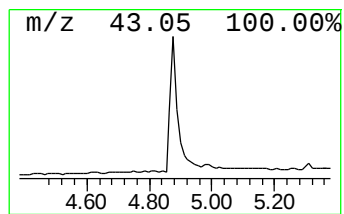
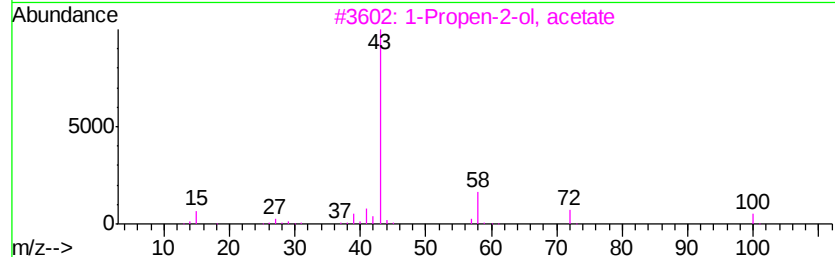
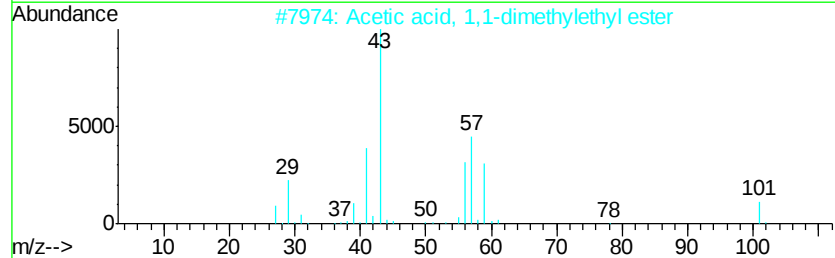
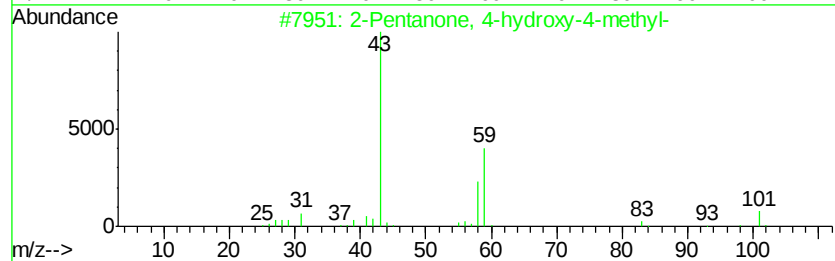
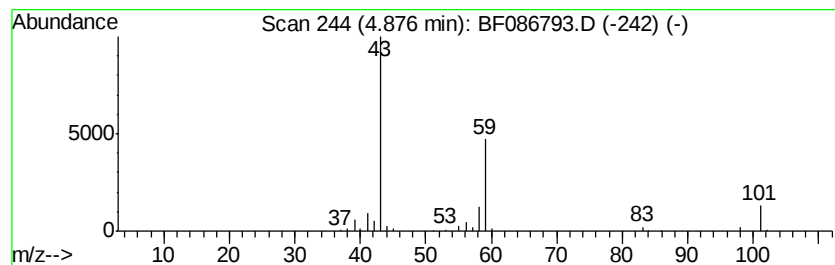
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	7.18 ng	199857	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			Butane	58	C4H10	000106-97-8	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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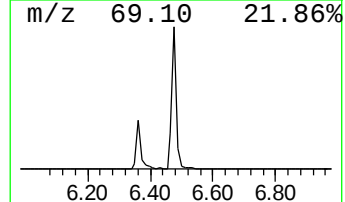
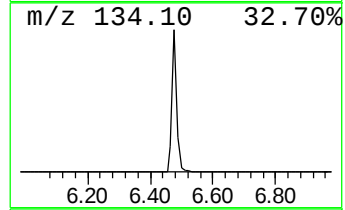
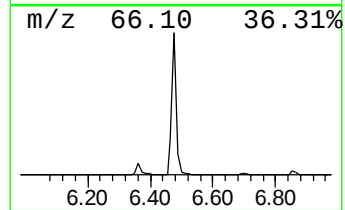
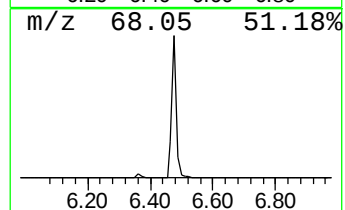
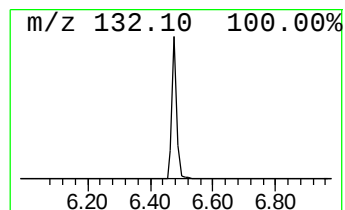
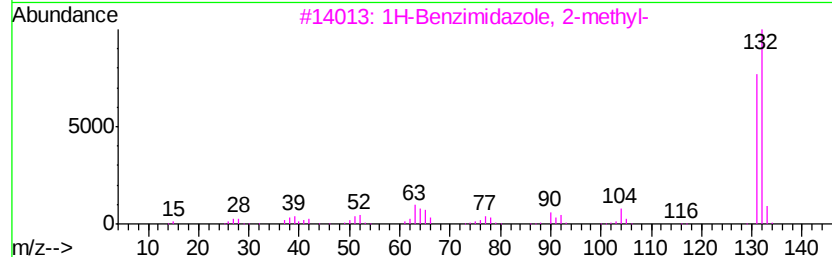
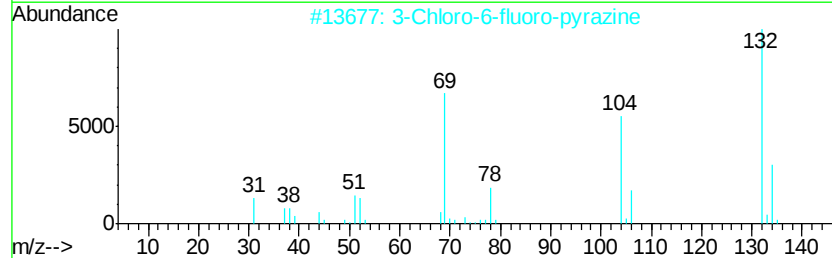
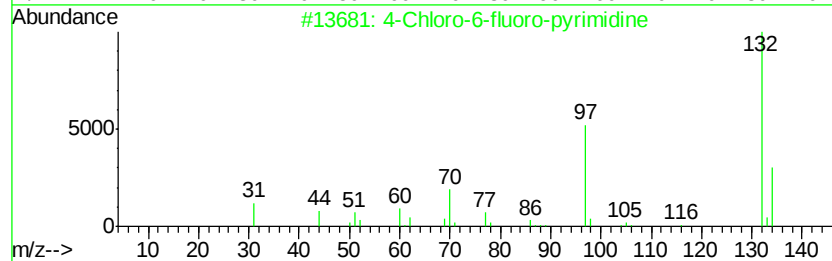
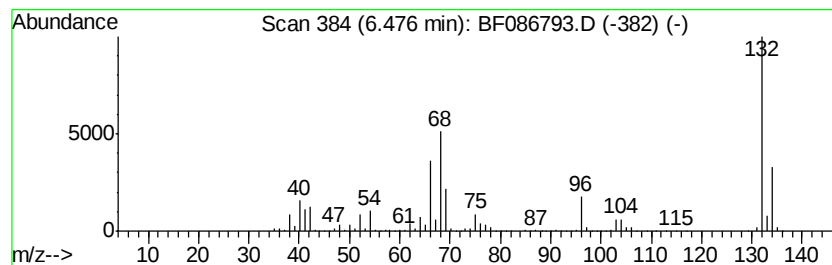
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	167.14 ng	4654620	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27		
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27		
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22		
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22		
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16		



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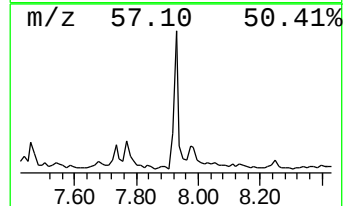
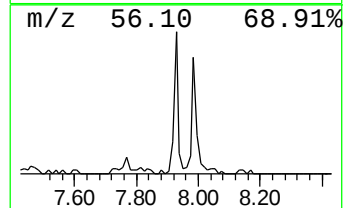
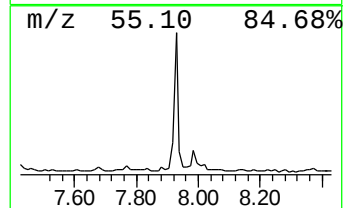
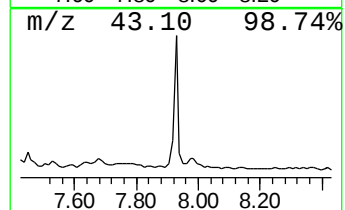
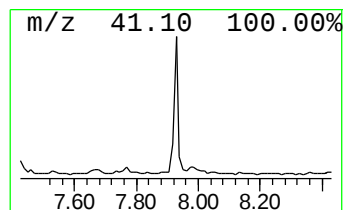
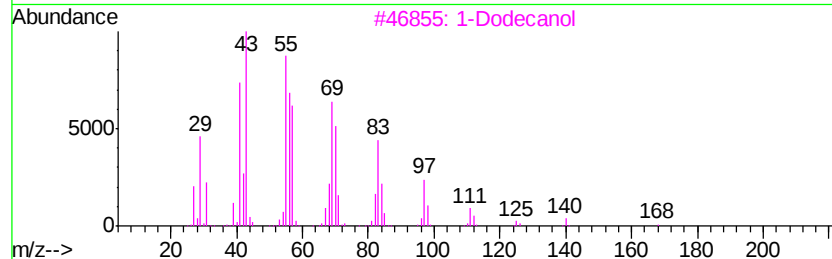
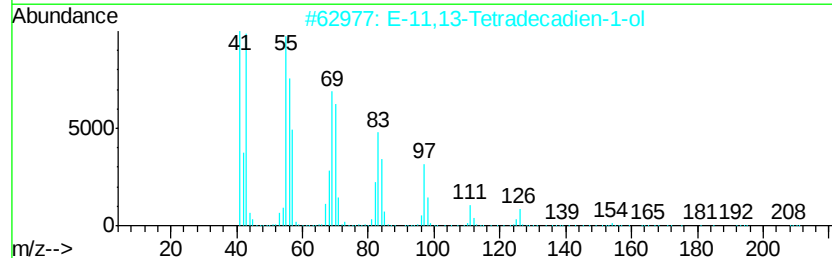
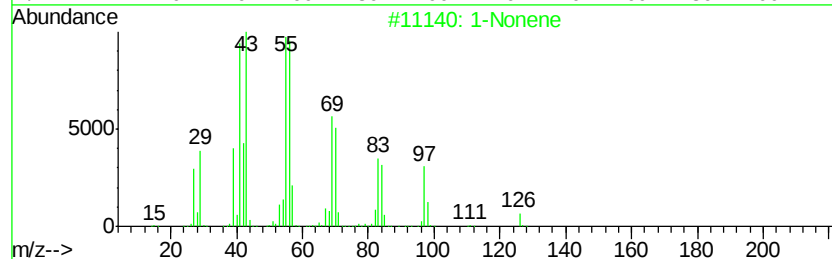
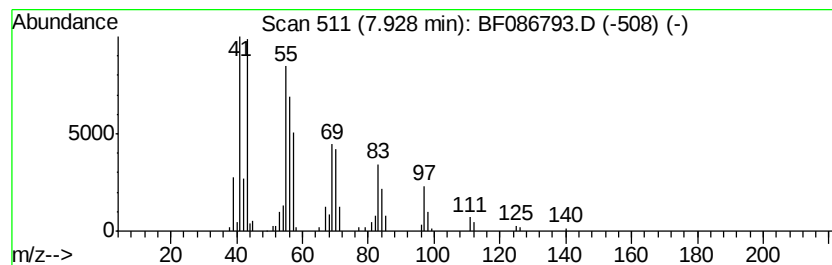
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Nonene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.93	4.14 ng	148342	Napthalene-d8	7.98

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonene		126	C9H18	000124-11-8	91
2	E-11,13-Tetradecadien-1-ol		210	C14H26O	1000131-00-3	90
3	1-Dodecanol		186	C12H26O	000112-53-8	90
4	Cyclopropane, octyl-		154	C11H22	001472-09-9	86
5	1-Dodecene		168	C12H24	000112-41-4	86



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ALS Vial : 63 Sample Multiplier: 1

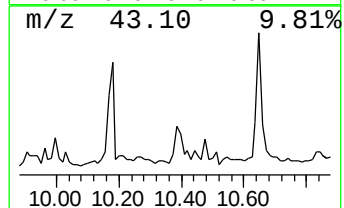
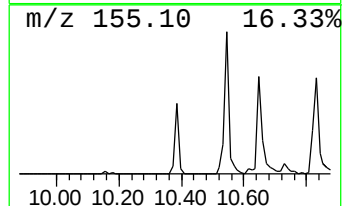
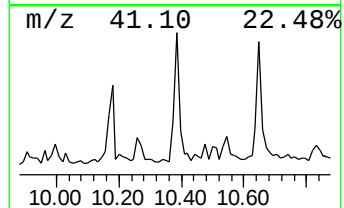
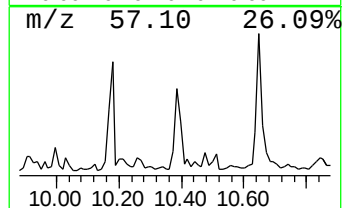
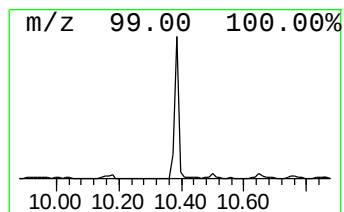
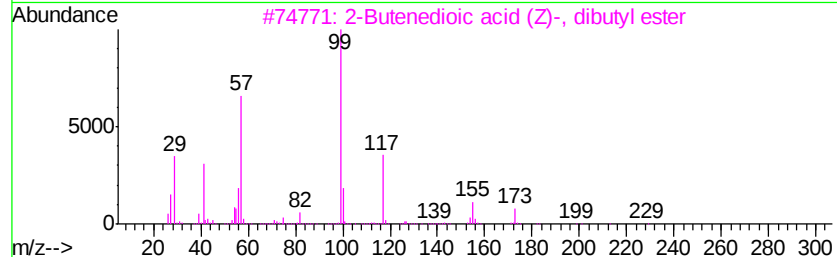
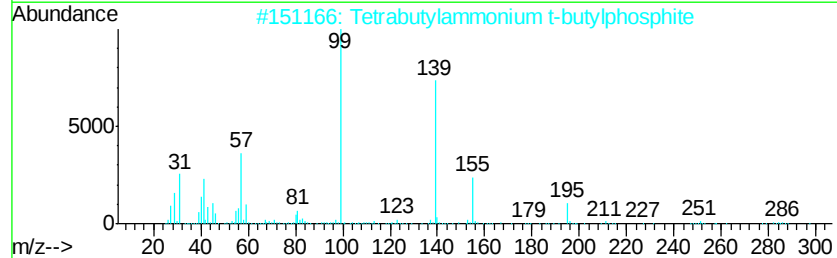
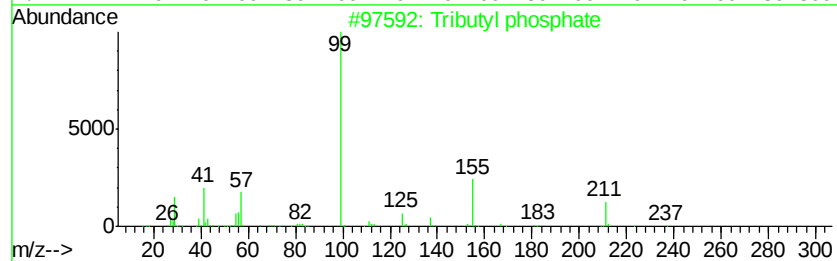
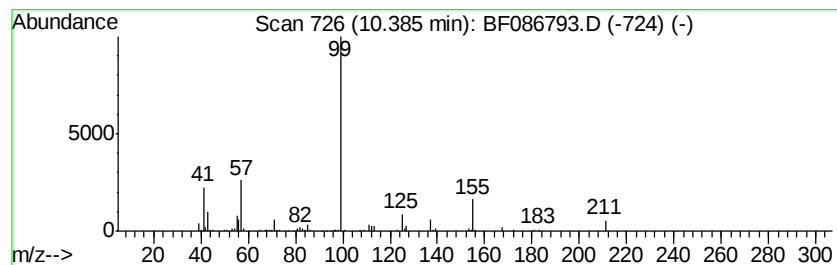
Instrument :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Tributyl phosphate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.38	4.84 ng	216590	Acenaphthene-d10	9.73	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tributyl phosphate	266	C12H27O4P	000126-73-8	90
2	Tetrabutylammonium t-butylphosphite	379	C20H46N03P	1000164-81-7	39
3	2-Butenedioic acid (Z)-, dibutyl...	228	C12H20O4	000105-76-0	38
4	(.+/-)-Dethiobiotin	214	C10H18N2O3	000636-20-4	38
5	n-Butyl methylphosphonofluoridate	154	C5H12F02P	000352-63-6	36



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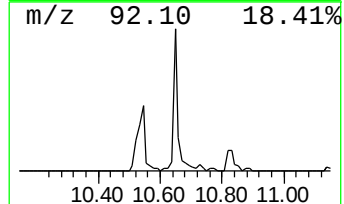
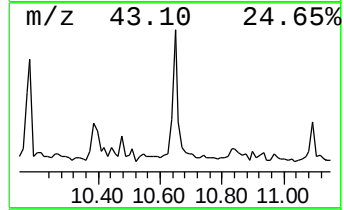
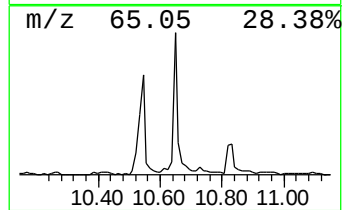
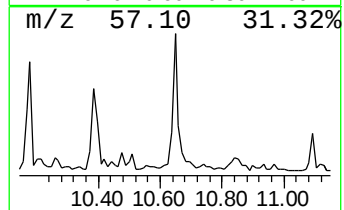
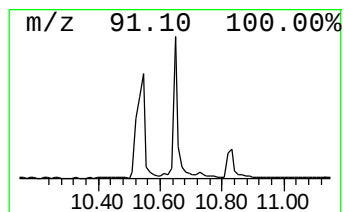
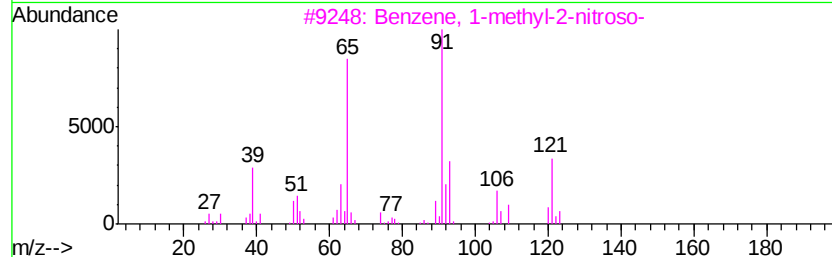
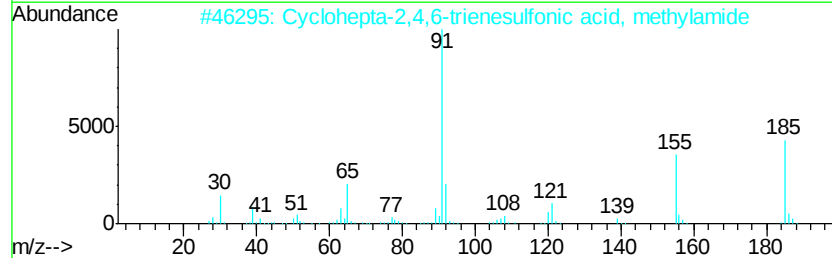
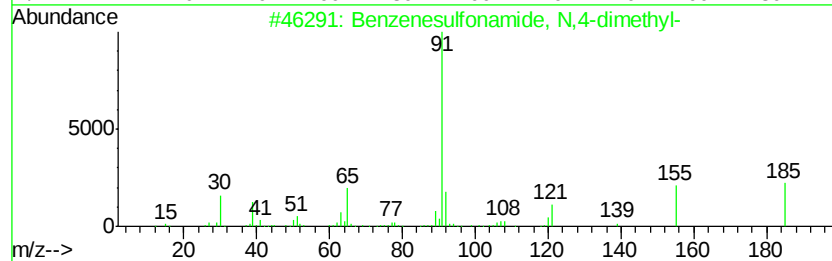
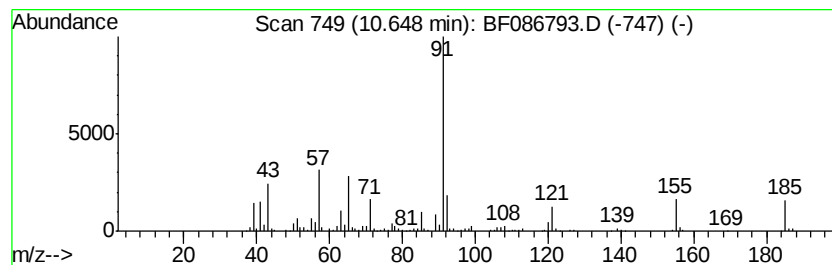
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzenesulfonamide, N,4-dim... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.65	12.65 ng	462436	Phenanthrene-d10	11.22		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	93
2		Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	70
3		Benzene, 1-methyl-2-nitroso-	121	C7H7NO	000611-23-4	58
4		1-Benzyl-3-hydroxypicolinic acid...	229	C13H11NO3	1000212-09-1	47
5		Benzeneacetaldehyde	120	C8H8O	000122-78-1	46



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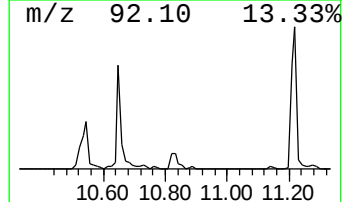
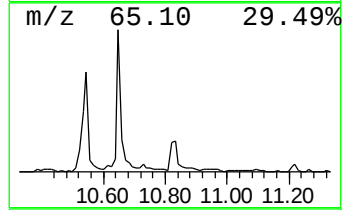
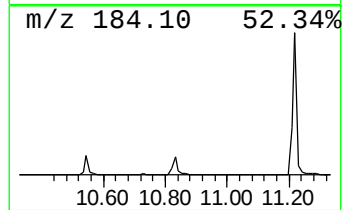
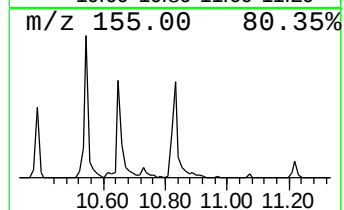
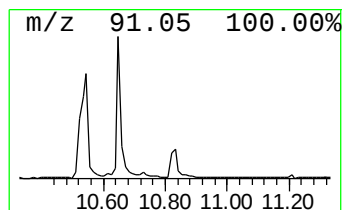
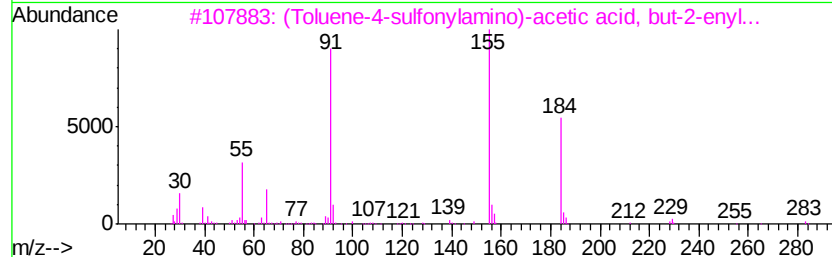
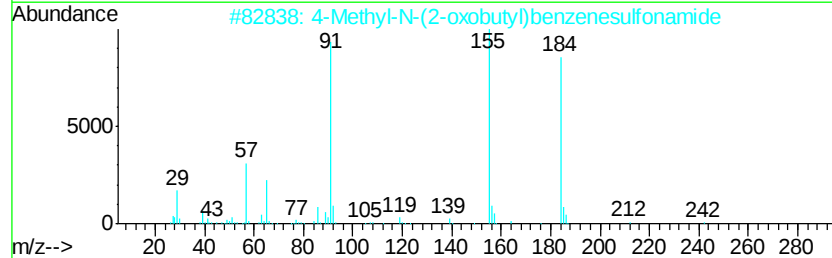
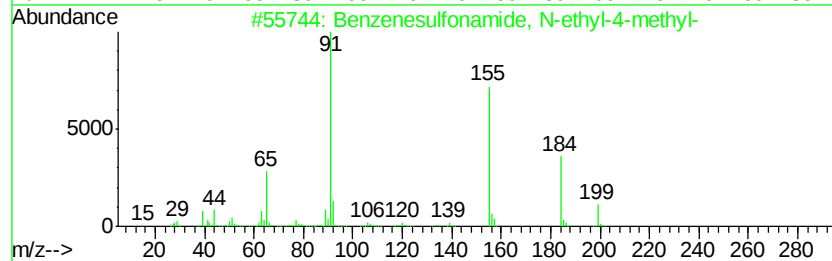
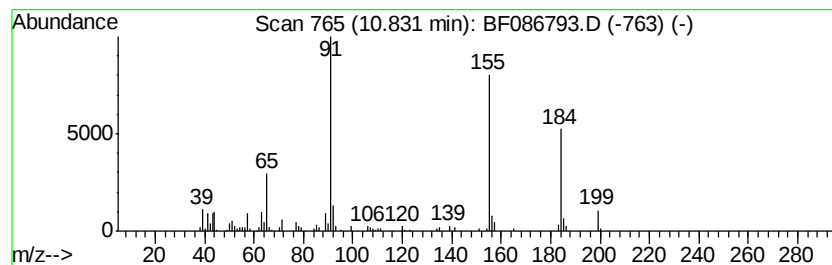
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzenesulfonamide, N-ethyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.83	4.22 ng	154180	Phenanthrene-d10	11.22		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzenesulfonamide, N-ethyl-4-me...	199	C9H13NO2S	000080-39-7	98
2		4-Methyl-N-(2-oxobutyl)benzenesu...	241	C11H15NO3S	1000192-14-5	90
3		(Toluene-4-sulfonylamino)-acetic...	283	C13H17NO4S	1000190-48-0	72
4		Pyridine-2-carbonitrile, 3,5,6-t...	375	C13H8Cl3N3O2S	255713-77-0	58
5		4-Toluenesulfonylmethylisocyanide	195	C9H9NO2S	036635-61-7	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
Data File : BF086793.D
Acq On : 8 May 2016 00:26
Operator : UM/SJ
Sample : H2882-05
Misc :
ALS Vial : 63 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MWHR4-9

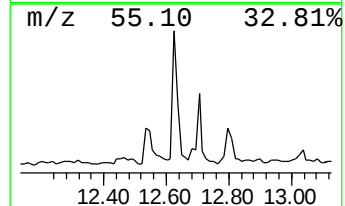
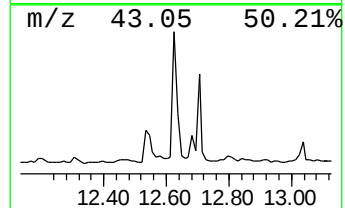
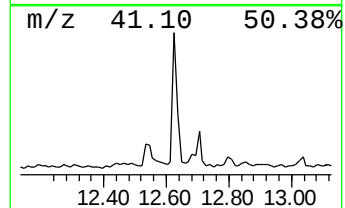
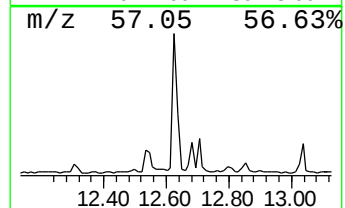
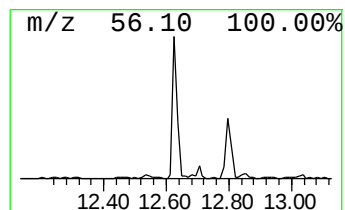
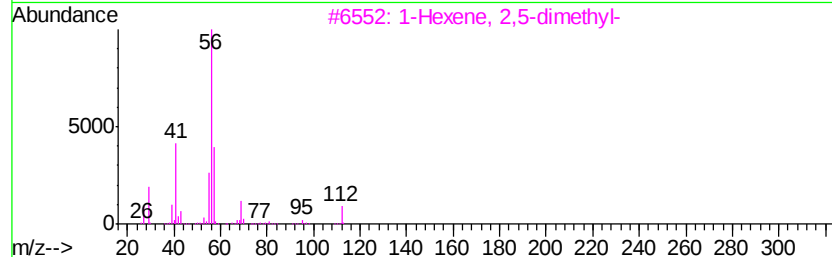
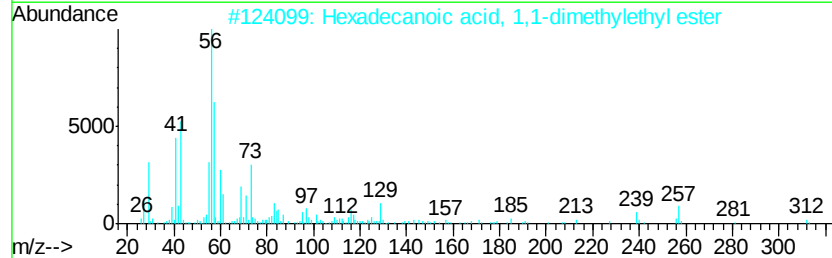
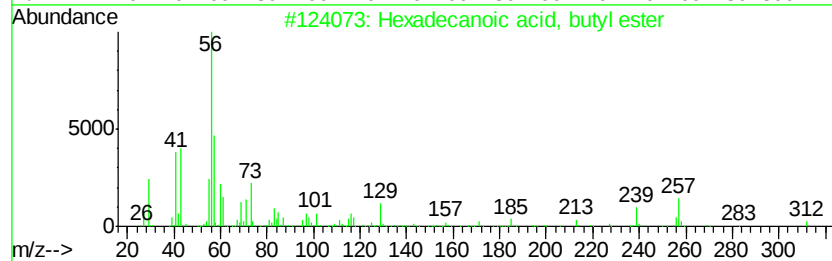
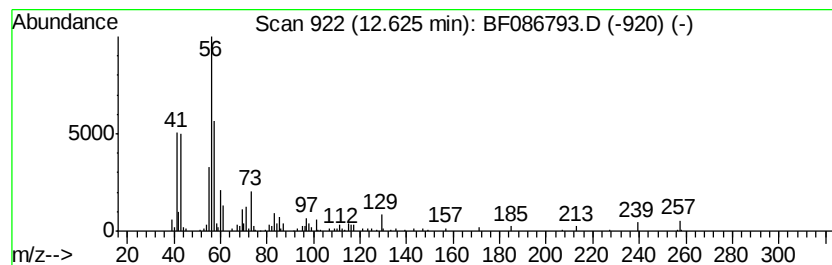
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	8.57 ng	226084	Chrysene-d12	13.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	50
3		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	38
4		Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	38
5		2-Isopropyl-3-vinylloxirane	112	C7H12O	070777-23-0	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
Data File : BF086793.D
Acq On : 8 May 2016 00:26
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ClientSampleId :
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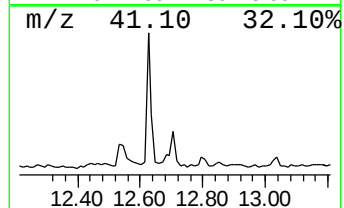
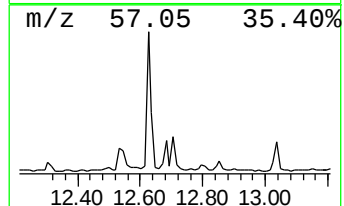
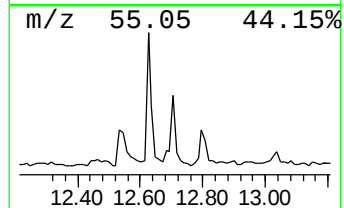
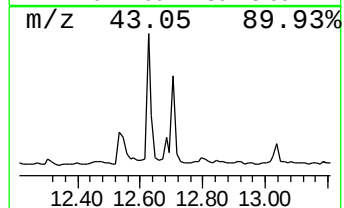
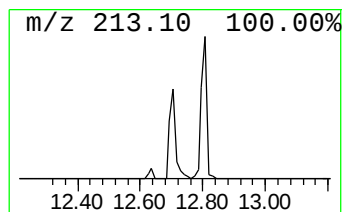
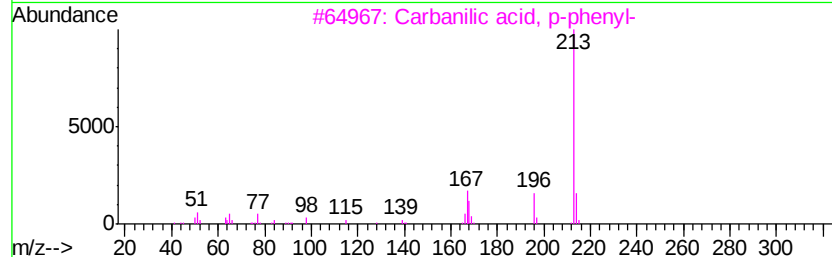
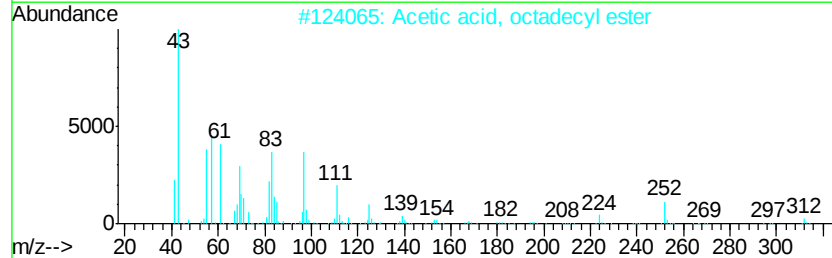
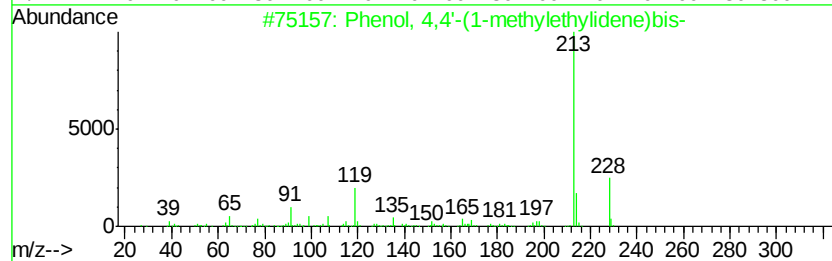
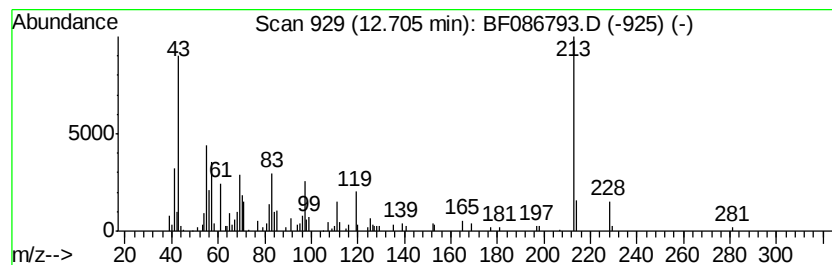
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Phenol, 4,4'-(1-methylethyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	5.07 ng	133756	Chrysene-d12	13.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	55	
2	Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	42	
3	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	41	
4	1-Hexadecanol, acetate	284	C18H36O2	000629-70-9	38	
5	1-Octadecanol	270	C18H38O	000112-92-5	35	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
Data File : BF086793.D
Acq On : 8 May 2016 00:26
Operator : UM/SJ
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Misc :
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ClientSampleId :
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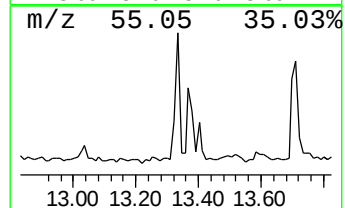
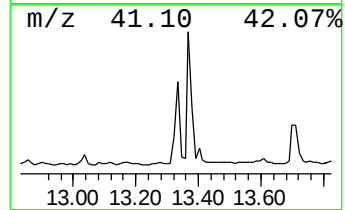
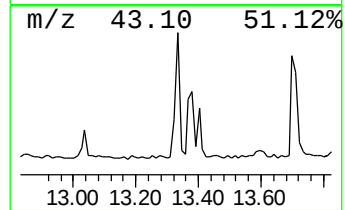
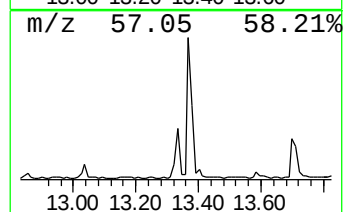
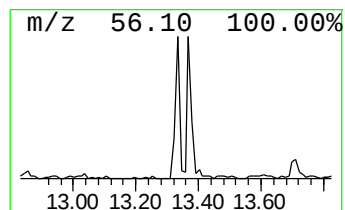
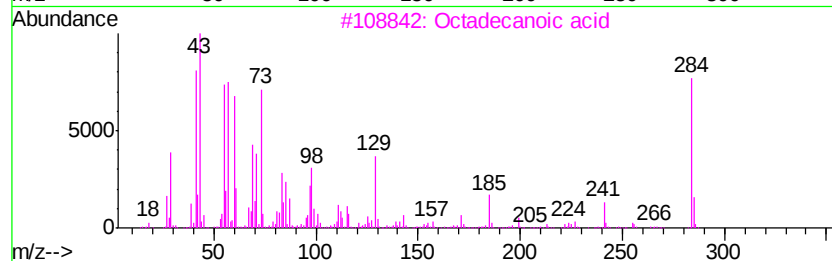
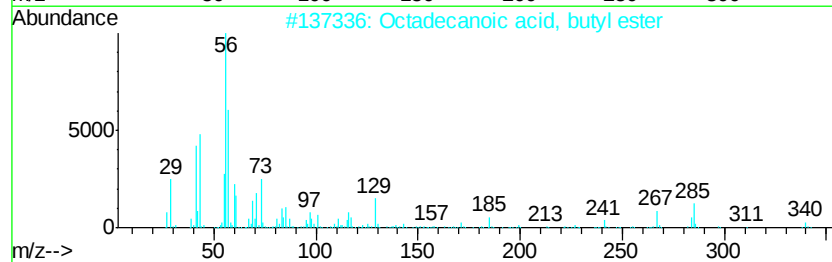
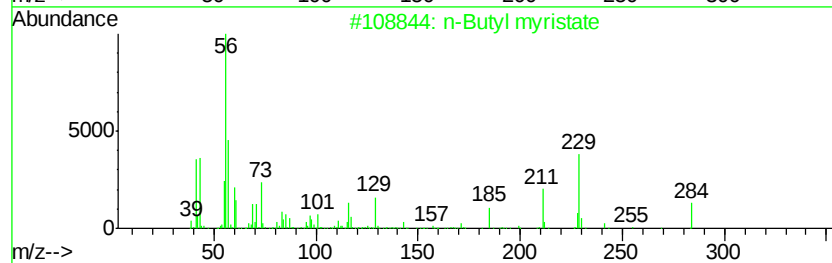
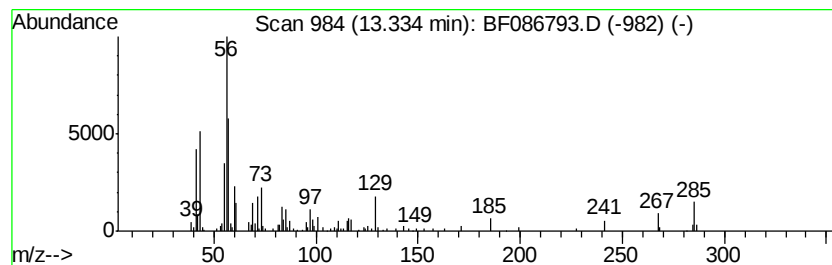
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 n-Butyl myristate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.33	5.68 ng	149861	Chrysene-d12	13.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Butyl myristate	284	C18H36O2	000110-36-1	80
2		Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	62
3		Octadecanoic acid	284	C18H36O2	000057-11-4	46
4		Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	38
5		Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	38



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Data File : BF086793.D
Acq On : 8 May 2016 00:26
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ClientSampleId :
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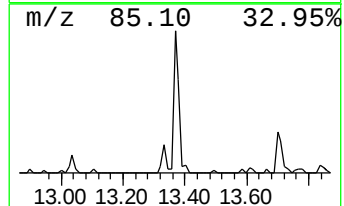
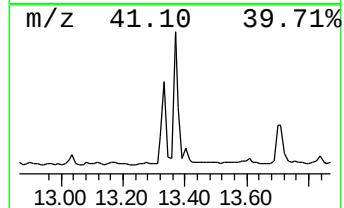
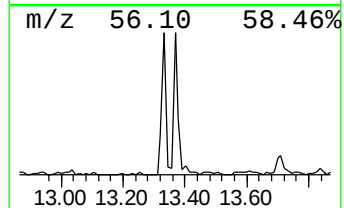
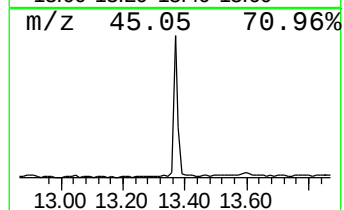
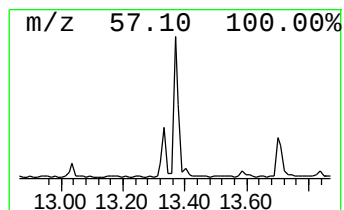
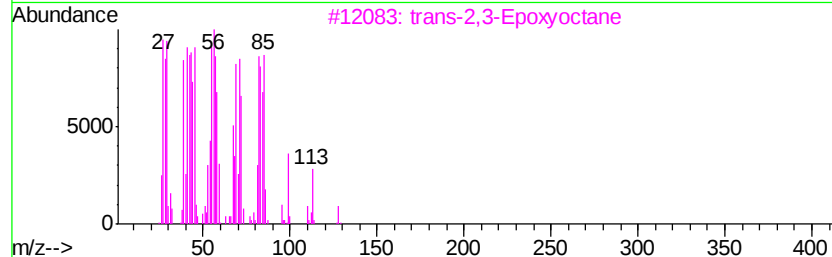
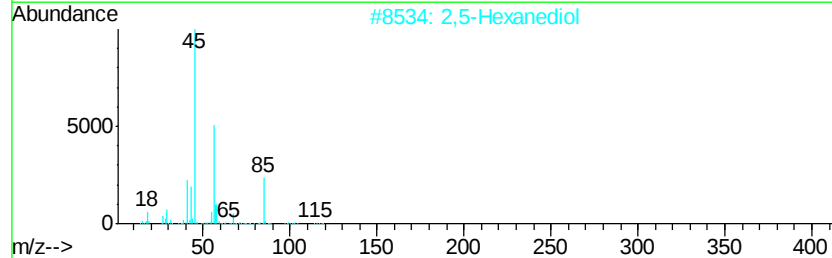
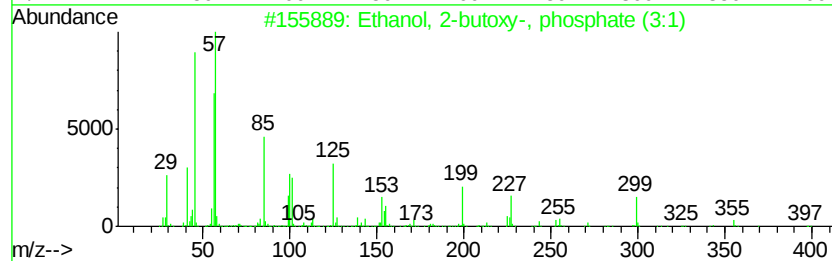
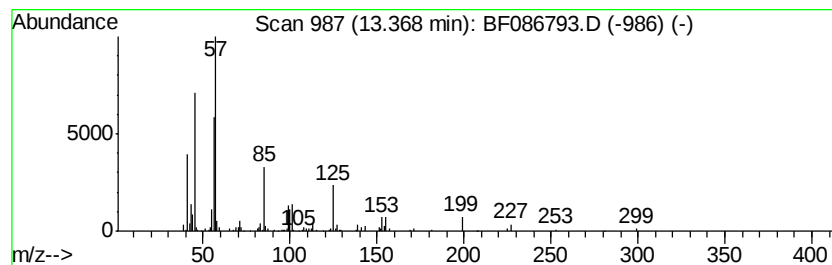
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Ethanol, 2-butoxy-, phospho... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.37	9.08 ng	239680	Chrysene-d12	13.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-butoxy-, phosphate (3:1)	398	C18H39O7P	000078-51-3	59
2			2,5-Hexanediol	118	C6H14O2	002935-44-6	47
3			trans-2,3-Epoxyoctane	128	C8H16O	028180-70-3	43
4			Furan, tetrahydro-2,5-dimethyl-	100	C6H12O	001003-38-9	35
5			2(3H)-Furanone, dihydro-5-methyl-	100	C5H8O2	000108-29-2	35



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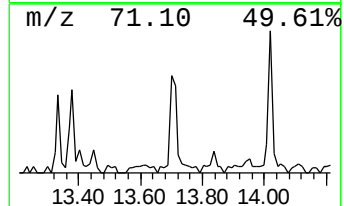
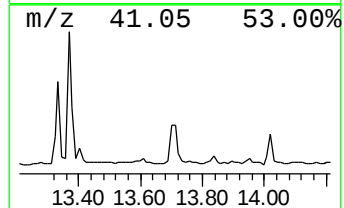
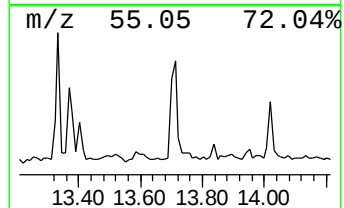
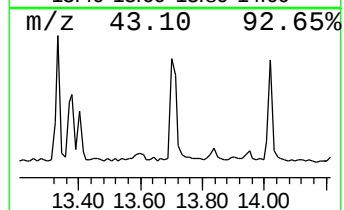
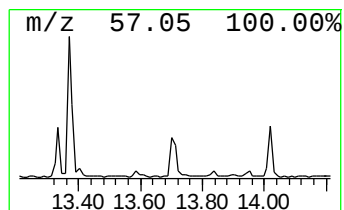
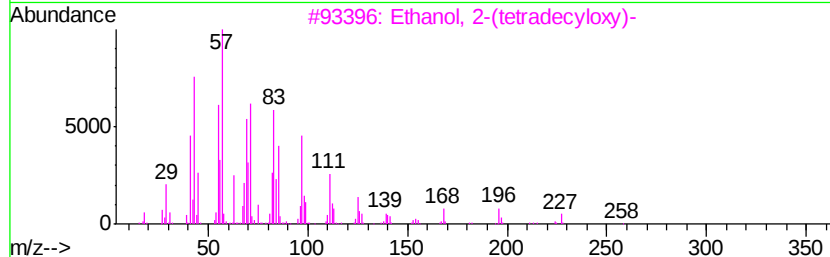
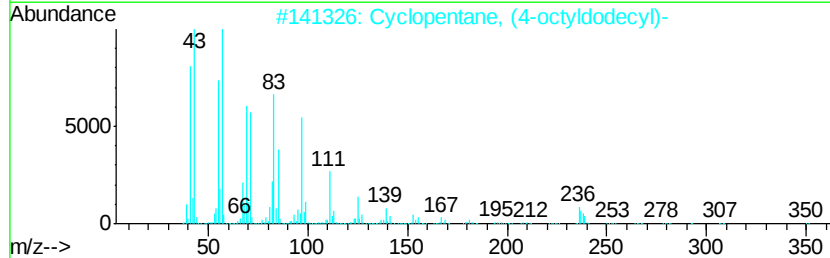
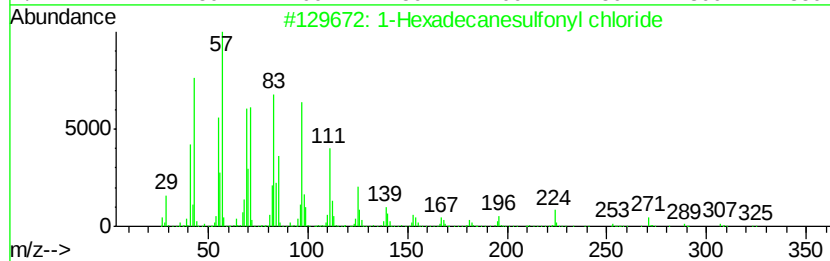
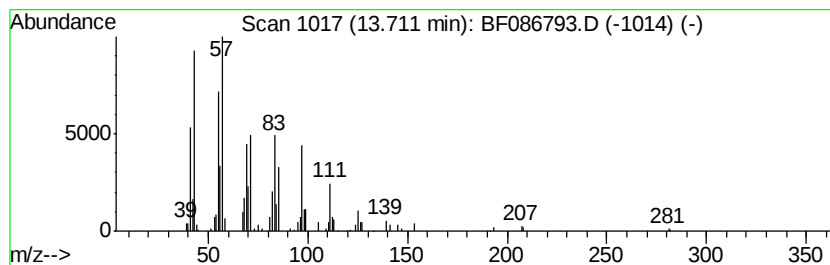
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Hexadecanesulfonyl chloride Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.71	5.35 ng	141287	Chrysene-d12	13.85		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
2		Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	87
3		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	83
4		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	81
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	76



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
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Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.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...	4.88	7.2	ng	199857	1	6.70	1113980	40.0
unknown6.48	6.48	167.1	ng	4654620	1	6.70	1113980	40.0
1-Nonene	7.93	4.1	ng	148342	2	7.98	1432470	40.0
Tributyl phosphate	10.38	4.8	ng	216590	3	9.73	1790120	40.0
Benzenesulfonamid...	10.65	12.7	ng	462436	4	11.22	1462520	40.0
Benzenesulfonamid...	10.83	4.2	ng	154180	4	11.22	1462520	40.0
Hexadecanoic acid...	12.63	8.6	ng	226084	5	13.85	1055410	40.0
Phenol, 4,4'-(1-m...	12.71	5.1	ng	133756	5	13.85	1055410	40.0
n-Butyl myristate	13.33	5.7	ng	149861	5	13.85	1055410	40.0
Ethanol, 2-butoxy...	13.37	9.1	ng	239680	5	13.85	1055410	40.0
1-Hexadecanesulfo...	13.71	5.3	ng	141287	5	13.85	1055410	40.0