

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
 Data File : BF092164.D
 Acq On : 10 Jan 2017 3:17
 Operator : UM/SJ
 Sample : I1055-03
 Misc :
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W-30

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-BF122116.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	4.767	249	252	262	rVB	313190	500578	15.29%	1.998%
2	5.247	292	294	303	rBV	1393594	1587352	48.47%	6.337%
3	6.287	382	385	386	rBV	382701	491201	15.00%	1.961%
4	6.310	386	387	394	rVB	717380	1078921	32.95%	4.307%
5	6.413	394	396	399	rBV	2355515	2947815	90.02%	11.767%
6	6.642	414	416	418	rBV	757243	766731	23.41%	3.061%
7	6.790	427	429	432	rBV	2007812	2632232	80.38%	10.508%
8	7.076	450	454	459	rVB3	15840	39014	1.19%	0.156%
9	7.213	463	466	468	rBV	1634337	1928918	58.90%	7.700%
10	7.922	526	528	531	rBV	650365	903418	27.59%	3.606%
11	8.939	615	617	620	rBV	59048	86265	2.63%	0.344%
12	9.008	620	623	625	rVV	3735130	3274679	100.00%	13.072%
13	9.110	628	632	633	rVV3	35313	37437	1.14%	0.149%
14	9.133	633	634	637	rVB	54541	54934	1.68%	0.219%
15	9.408	656	658	660	rVB	266212	225657	6.89%	0.901%
16	9.682	679	682	684	rBV	996159	977841	29.86%	3.903%
17	9.911	700	702	704	rBV2	25356	39975	1.22%	0.160%
18	10.105	713	719	726	rBV5	44382	125342	3.83%	0.500%
19	10.471	748	751	754	rBV	1837513	1769846	54.05%	7.065%
20	10.539	754	757	760	rVV	36785	62611	1.91%	0.250%
21	10.596	760	762	766	rVB2	126794	152633	4.66%	0.609%
22	11.065	799	803	805	rBV2	65155	138790	4.24%	0.554%
23	11.156	809	811	814	rBV	887709	887357	27.10%	3.542%
24	11.374	828	830	836	rBV3	34594	73581	2.25%	0.294%
25	11.716	857	860	863	rBV3	73364	149497	4.57%	0.597%
26	11.888	873	875	878	rVB4	20133	42484	1.30%	0.170%
27	12.116	893	895	899	rVB2	25398	54033	1.65%	0.216%
28	12.196	899	902	906	rBV2	17000	46613	1.42%	0.186%
29	12.482	925	927	929	rBV2	36142	67976	2.08%	0.271%
30	12.528	929	931	933	rVB	46704	52788	1.61%	0.211%
31	12.642	938	941	944	rBV2	31839	62014	1.89%	0.248%
32	12.745	948	950	953	rBV	2581795	2739479	83.66%	10.936%
33	13.317	998	1000	1002	rBV3	39855	65637	2.00%	0.262%
34	13.797	1039	1042	1044	rBV	462300	580389	17.72%	2.317%

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ALS Vial : 30 Sample Multiplier: 1

Instrument :
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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

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35	15.168	1160	1162	1164	rBV	326497	406885	12.43%	1.624%
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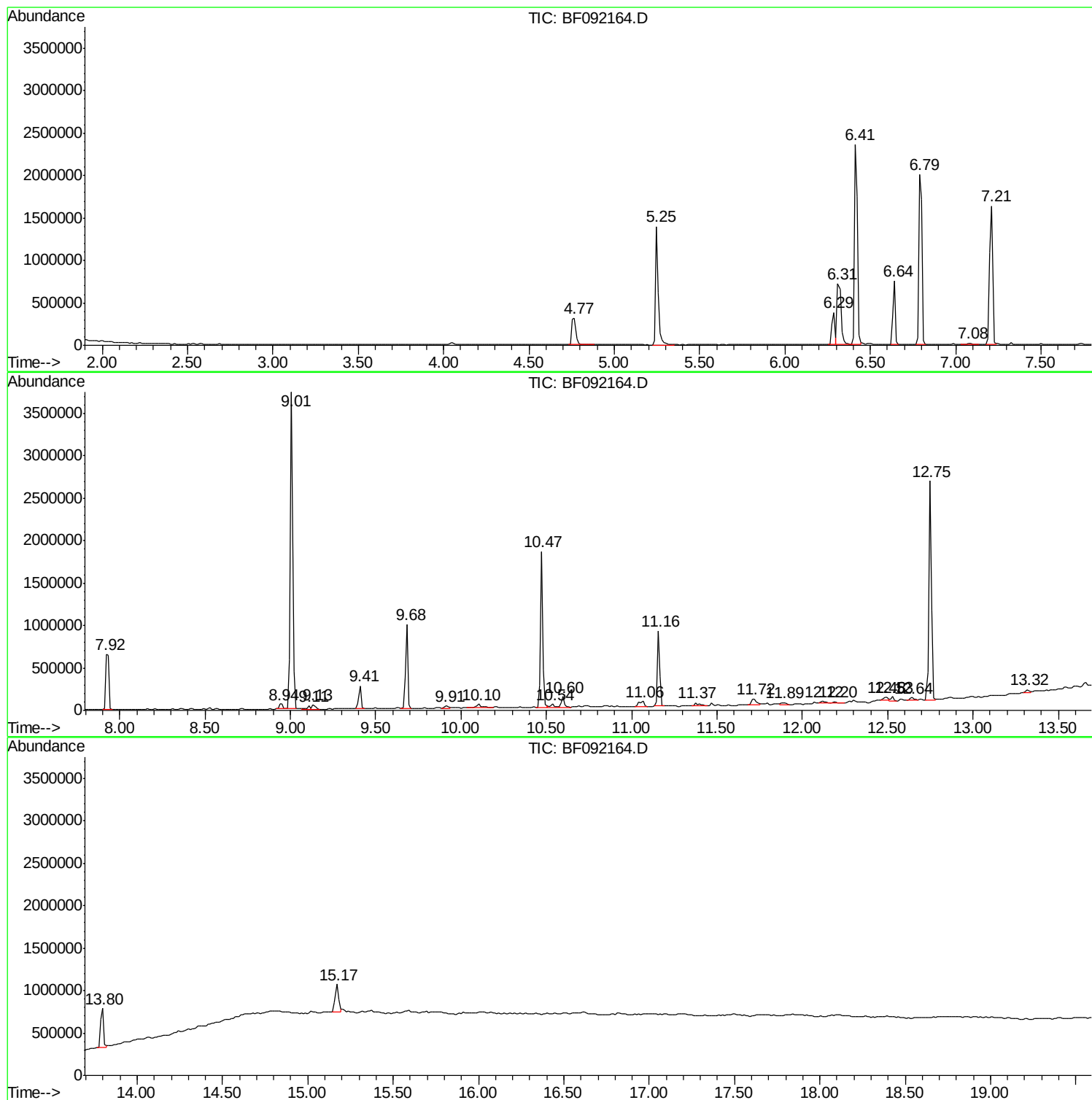
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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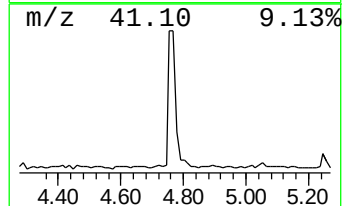
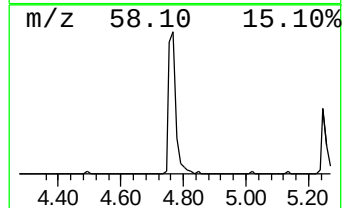
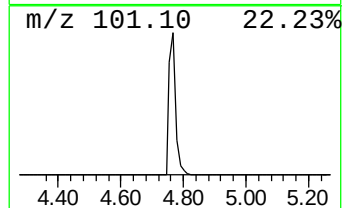
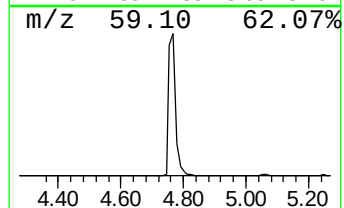
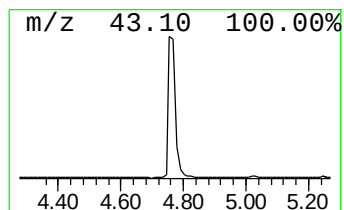
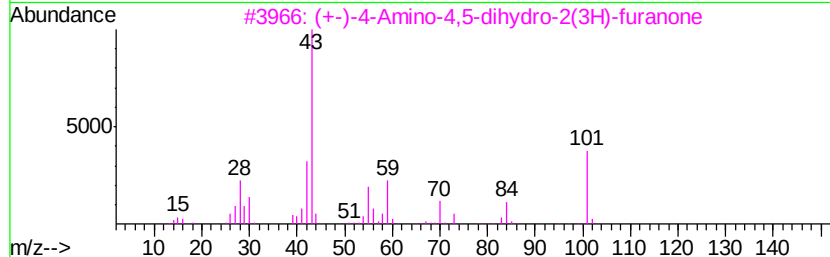
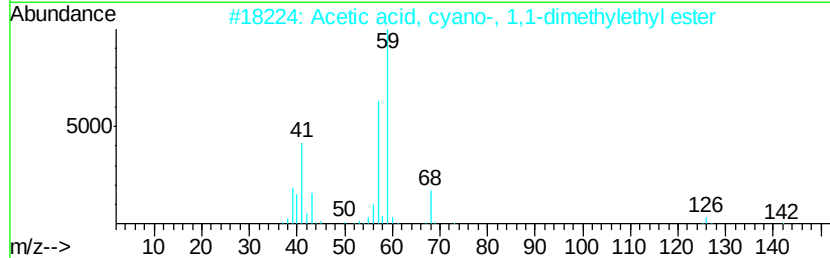
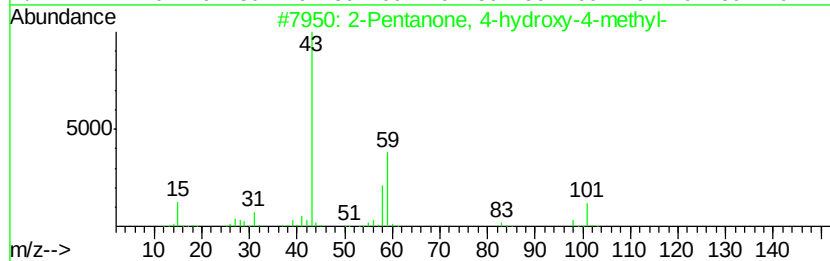
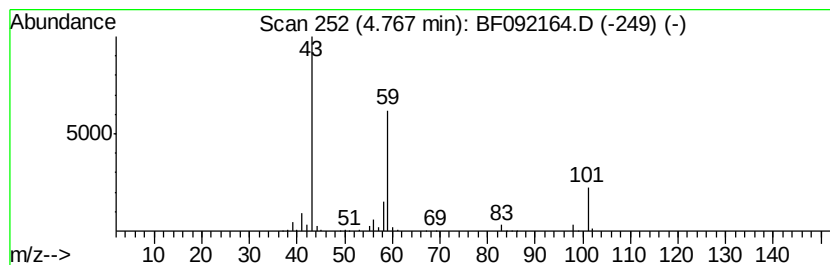
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.77	13.06 ng	500578	1,4-Dichlorobenzene-d4	6.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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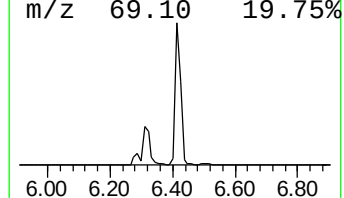
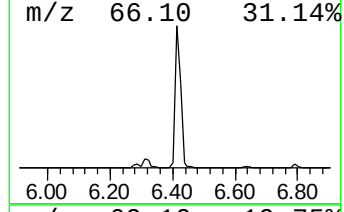
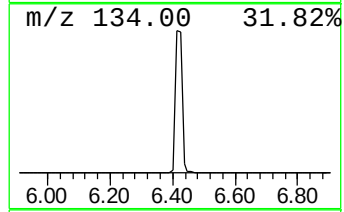
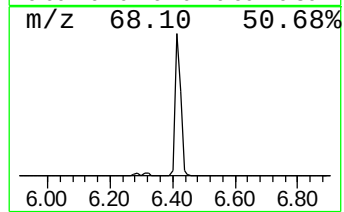
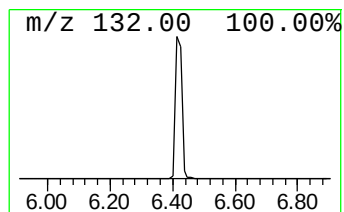
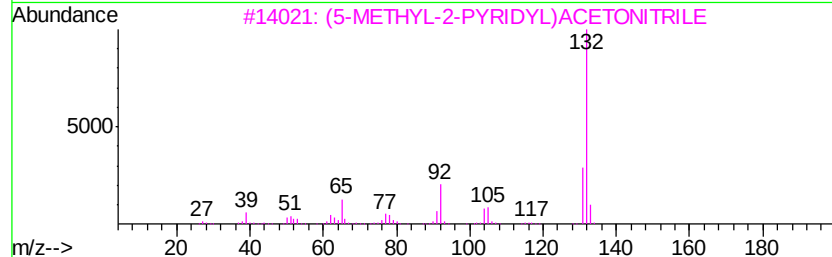
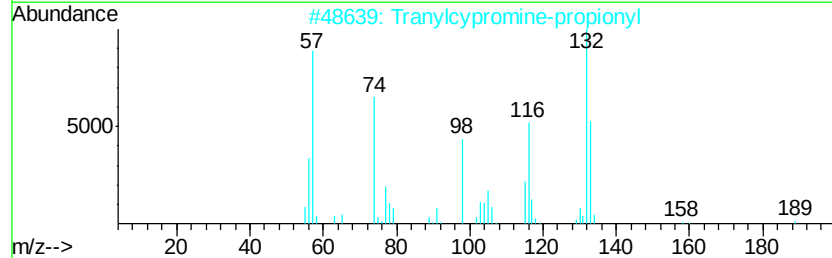
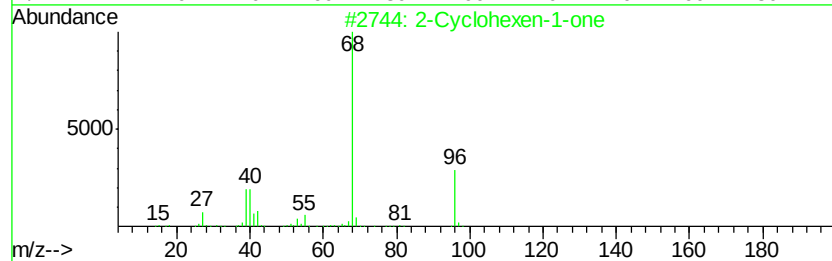
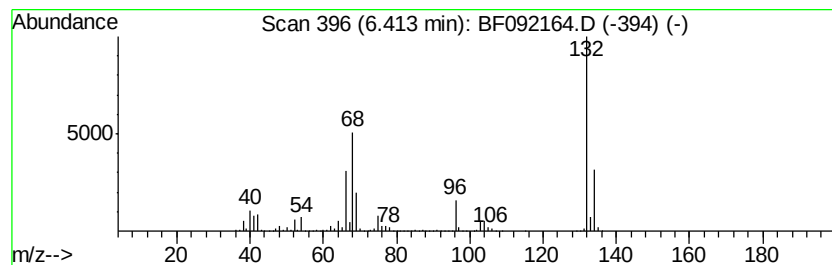
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.41 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.41	76.89 ng	2947820	1,4-Dichlorobenzene-d4	6.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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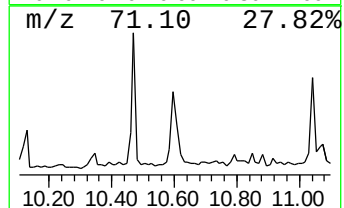
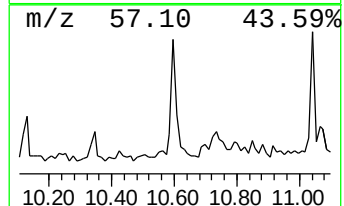
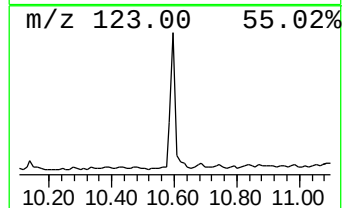
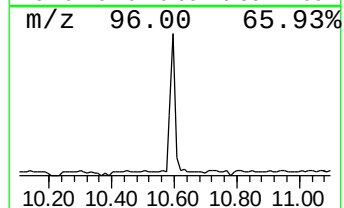
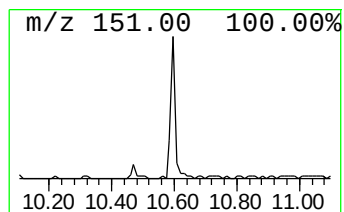
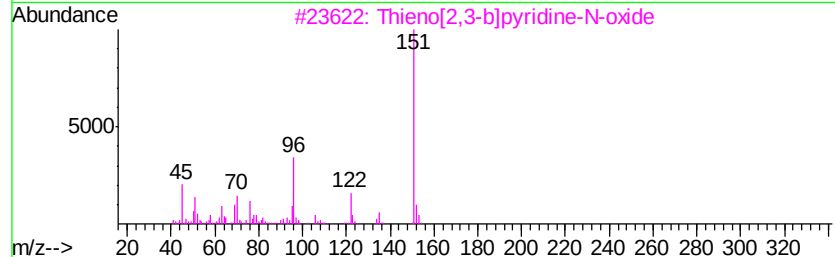
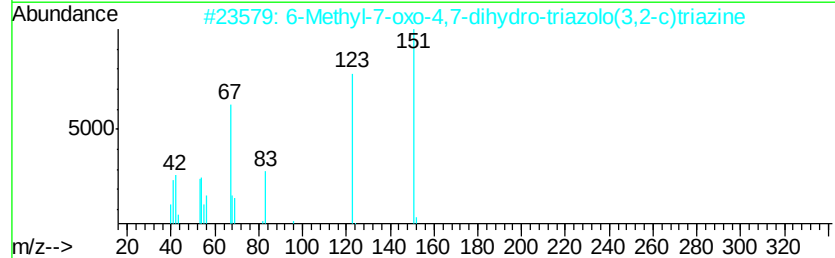
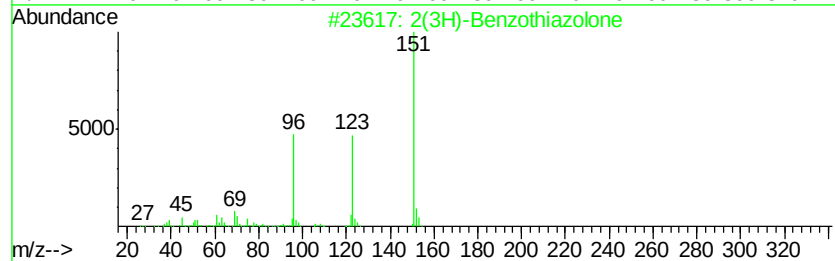
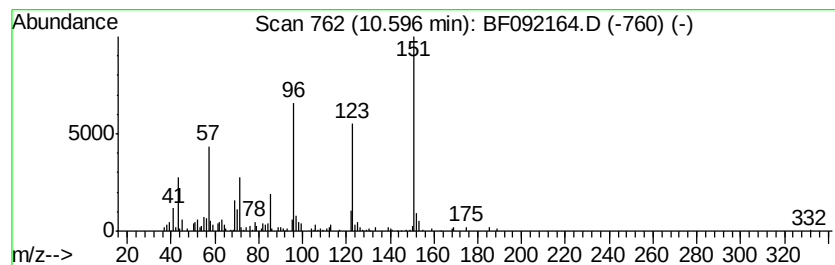
Instrument :
BNA_F
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 2(3H)-Benzothiazolone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.60	3.44 ng	152633	Phenanthrene-d10	11.16
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		2(3H)-Benzothiazolone	151 C7H5NOS	000934-34-9 87
2		6-Methyl-7-oxo-4,7-dihydro-triaz...	151 C5H5N5O	057250-39-2 47
3		Thieno[2,3-b]pyridine-N-oxide	151 C7H5NOS	025557-50-0 46
4		4-Mercaptoimidazo[4,5-c]pyridine	151 C6H5N3S	034550-51-1 38
5		2(3H)-Benzoxazolethione	151 C7H5NOS	002382-96-9 38



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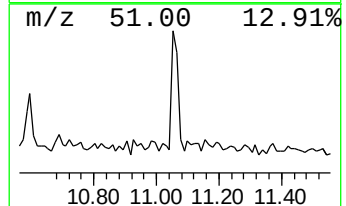
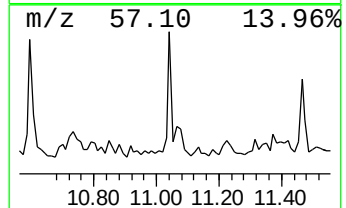
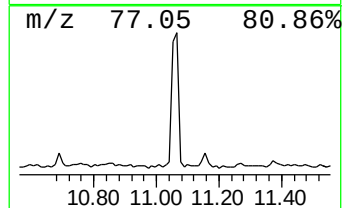
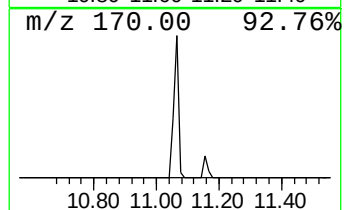
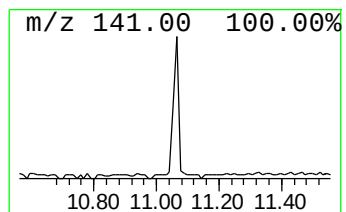
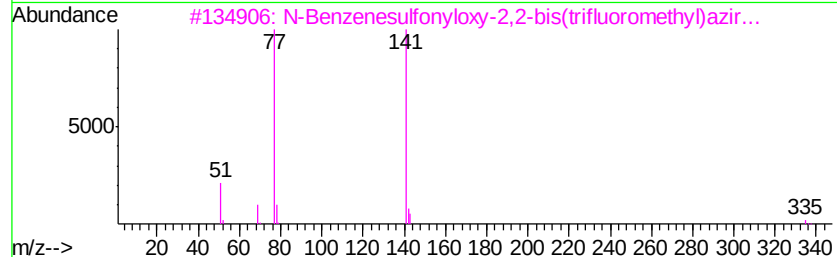
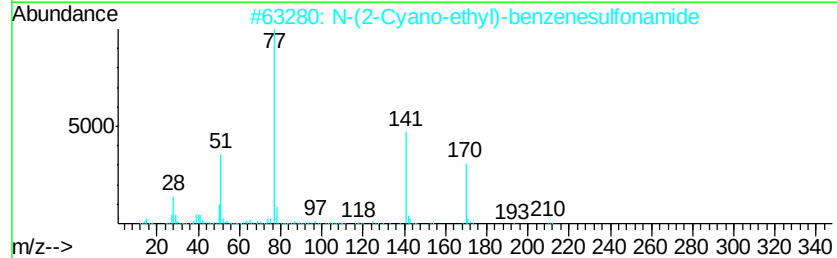
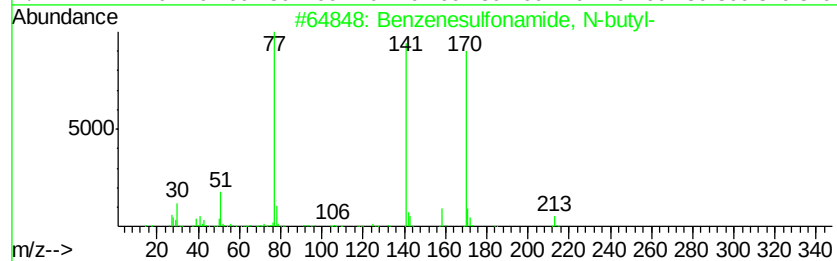
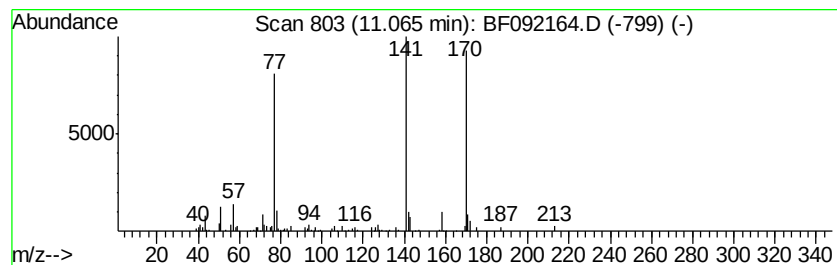
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzenesulfonamide, N-butyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.06	3.13 ng	138790	Phenanthrene-d10	11.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenesulfonamide, N-butyl-	213	C10H15NO2S	003622-84-2	91
2		N-(2-Cyano-ethyl)-benzenesulfona...	210	C9H10N2O2S	002619-21-8	78
3		N-Benzenesulfonyloxy-2,2-bis(tri...	335	C10H7F6N03S	055734-41-3	28
4		(Phenylsulfonyl)acetonitrile	181	C8H7N02S	007605-28-9	28
5		Benzenemethanol, 2-chloro-.alpha...	156	C8H9ClO	013524-04-4	28



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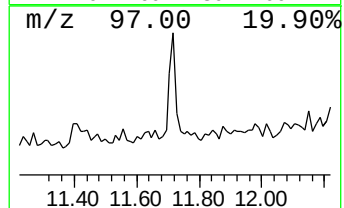
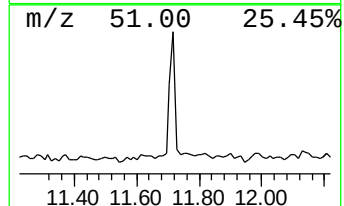
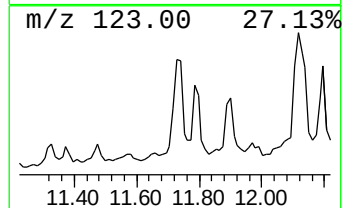
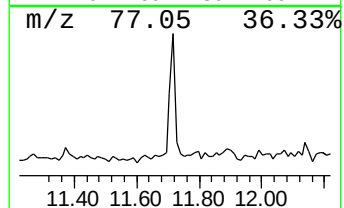
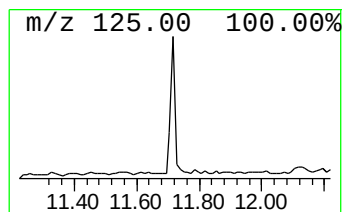
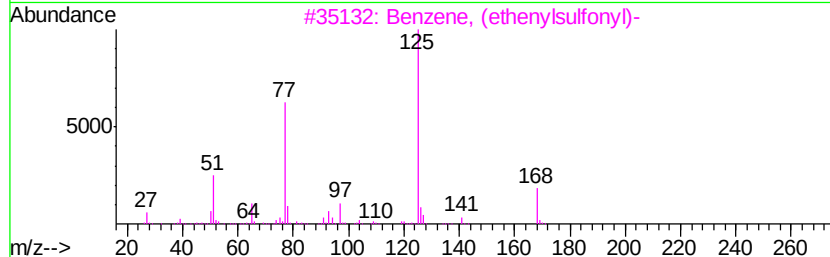
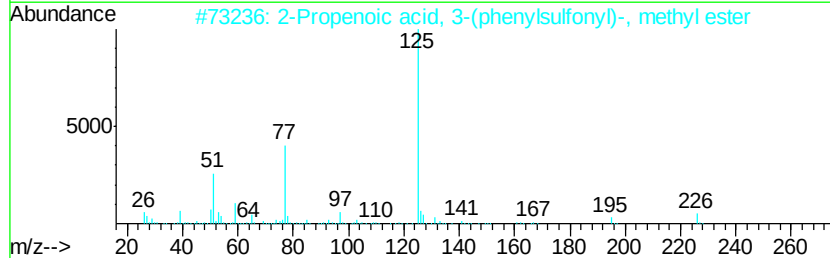
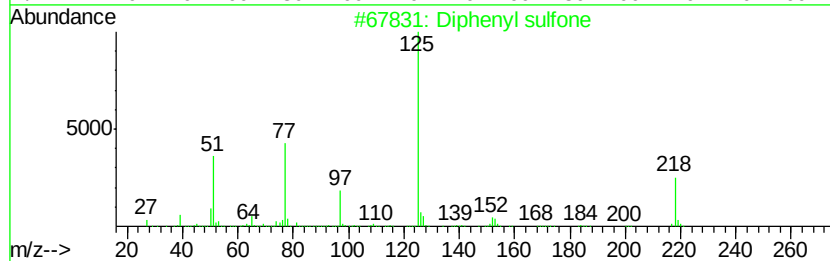
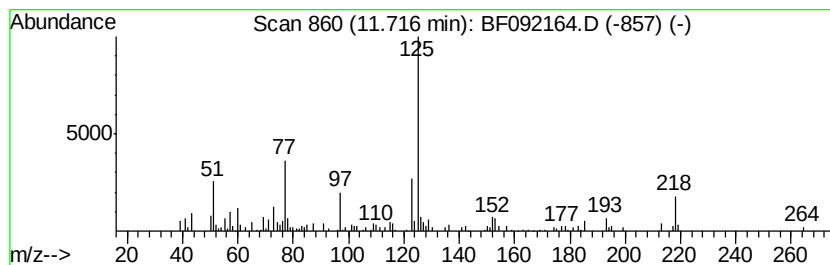
Instrument :
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ClientSampled :
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Diphenyl sulfone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.72	3.37 ng	149497	Phenanthrene-d10		11.16
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diphenyl sulfone	218	C12H10O2S	000127-63-9	93
2	2-Propenoic acid, 3-(phenylsulfo...	226	C10H10O4S	063068-63-3	47
3	Benzene, (ethenylsulfonyl)-	168	C8H8O2S	005535-48-8	43
4	Bis[phenylsulfonyl]-4-trichlorom...	522	C20H14Cl4O4S2	081269-12-7	42
5	Thiophene, 3-(1,1-dimethylethyl)-	140	C8H12S	001689-79-8	38



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ClientSampleId :
W-30

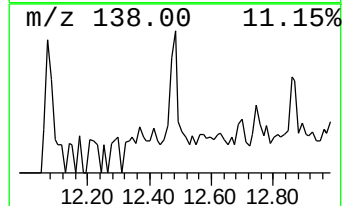
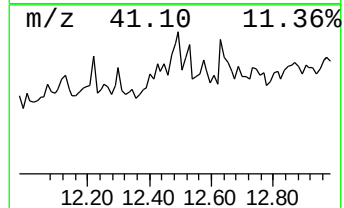
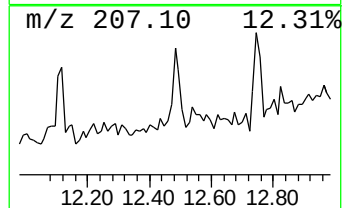
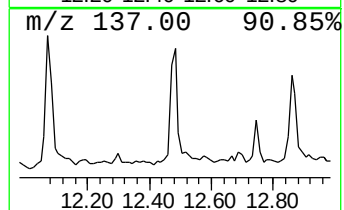
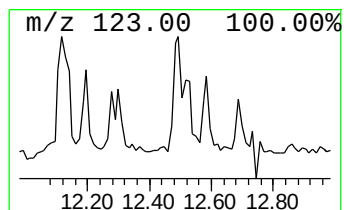
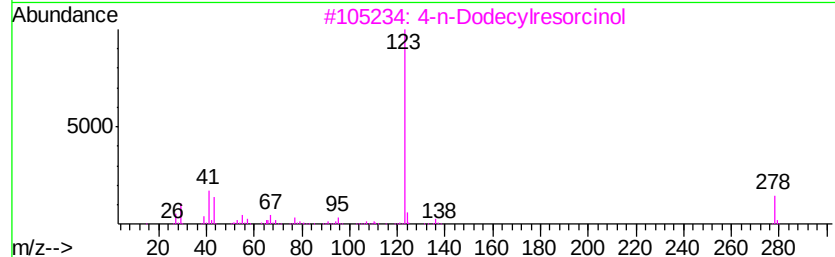
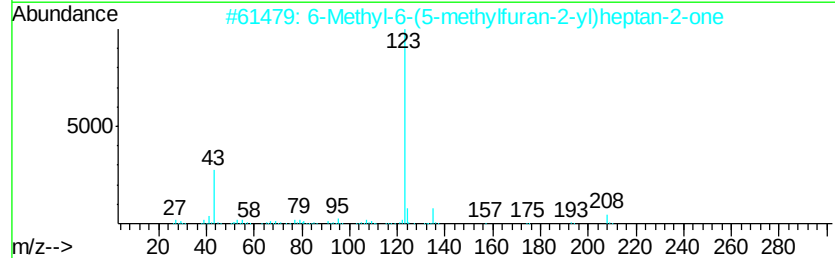
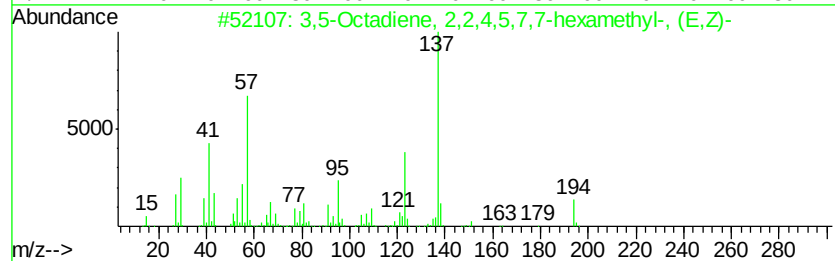
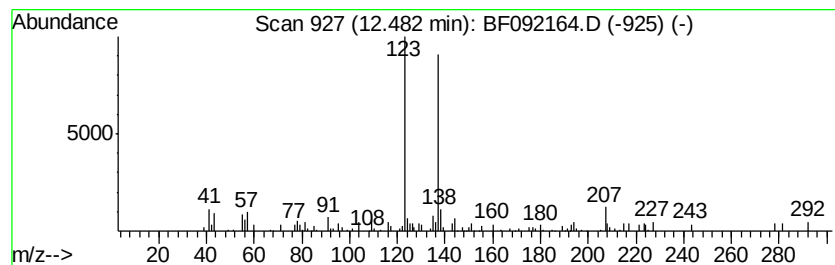
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown12.48 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	2.34 ng	67976	Chrysene-d12	13.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,5-Octadiene, 2,2,4,5,7,7-hexam...	194	C14H26	055712-52-2	32
2		6-Methyl-6-(5-methylfuran-2-yl)h...	208	C13H20O2	050464-95-4	27
3		4-n-Dodecylresorcinol	278	C18H30O2	024305-56-4	27
4		1,3-Benzenediol, 4-ethyl-	138	C8H10O2	002896-60-8	27
5		4-Hexanoylresorcinol	208	C12H16O3	003144-54-5	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
Data File : BF092164.D
Acq On : 10 Jan 2017 3:17
Operator : UM/SJ
Sample : I1055-03
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-30

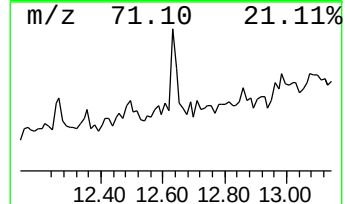
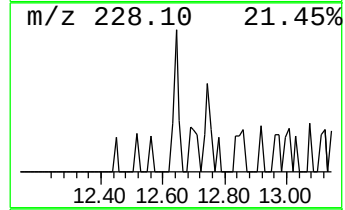
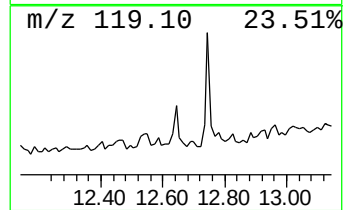
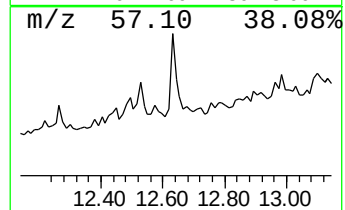
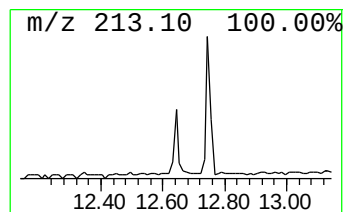
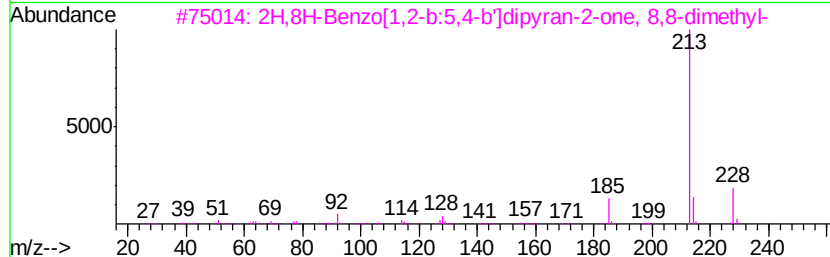
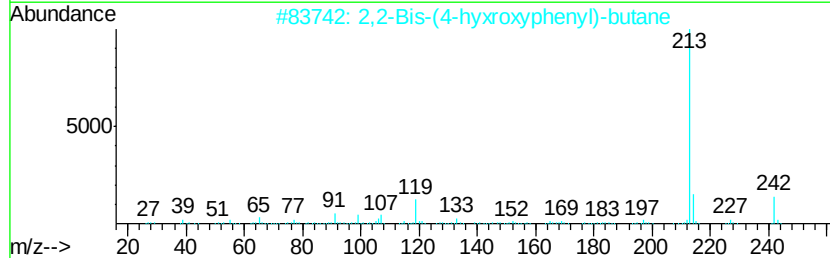
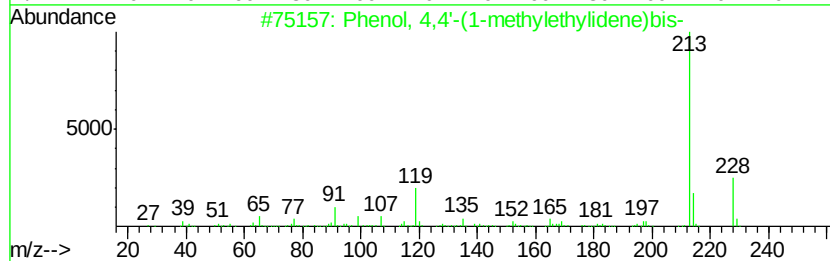
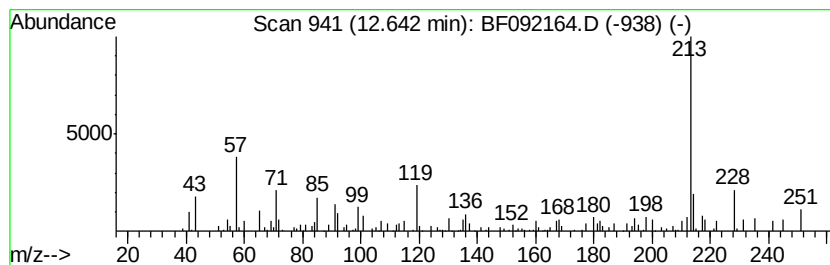
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Phenol, 4,4'-(1-methylethyl... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	2.14 ng	62014	Chrysene-d12	13.80

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	81	
2	2,2-Bis-(4-hydroxyphenyl)-butane	242	C16H18O2	000077-40-7	50	
3	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	50	
4	N-Benzyl-p-anisidine	213	C14H15NO	017377-95-6	46	
5	Carbamic acid, [1,1'-biphenyl]-3...	213	C13H11NO2	055030-29-0	46	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
Data File : BF092164.D
Acq On : 10 Jan 2017 3:17
Operator : UM/SJ
Sample : I1055-03
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
W-30

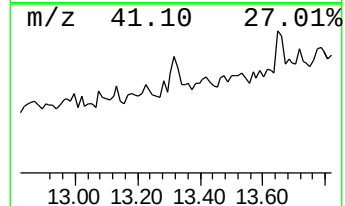
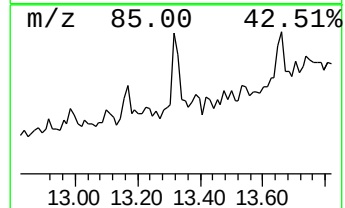
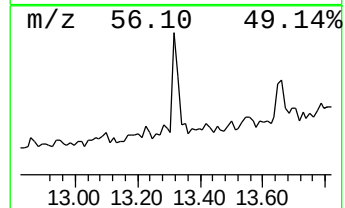
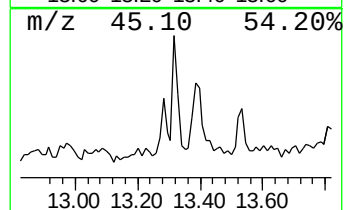
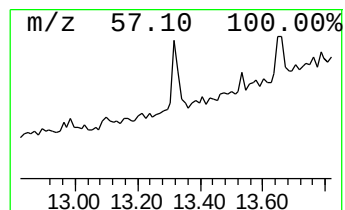
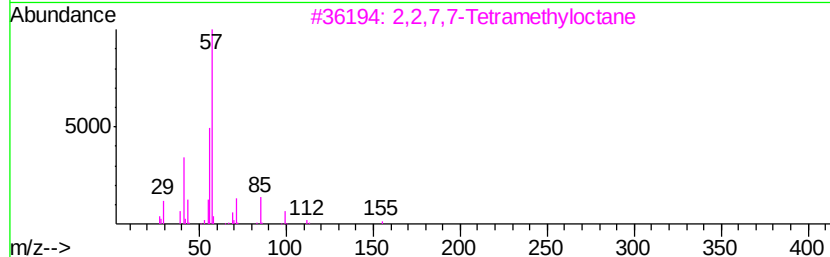
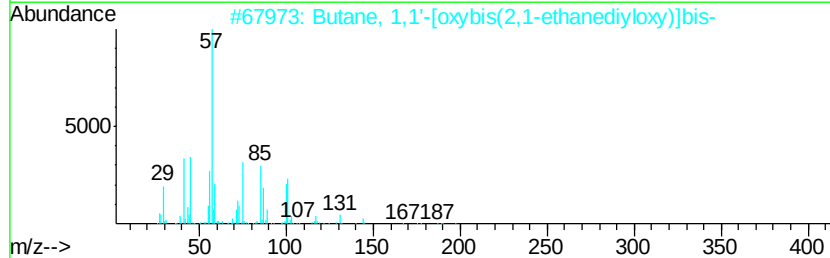
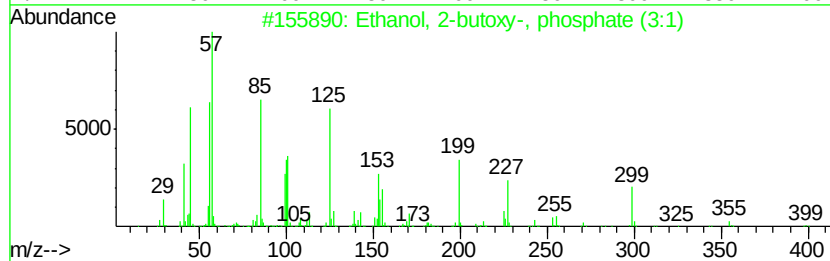
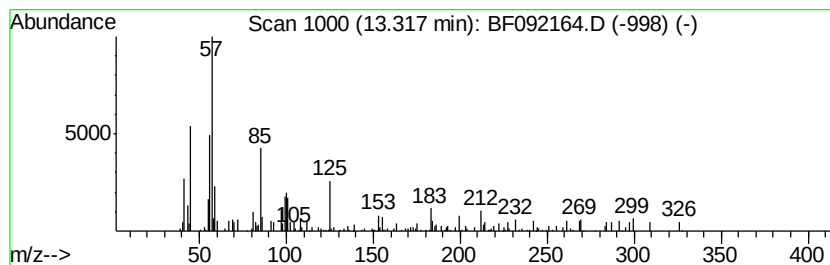
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Ethanol, 2-butoxy-, phospho... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.32	2.26 ng	65637	Chrysene-d12	13.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-butoxy-, phosphate (3:1)	398	C18H39O7P	000078-51-3	68
2		Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	38
3		2,2,7,7-Tetramethyloctane	170	C12H26	001071-31-4	16
4		Dodecane, 3-methyl-	184	C13H28	017312-57-1	14
5		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
Data File : BF092164.D
Acq On : 10 Jan 2017 3:17
Operator : UM/SJ
Sample : I1055-03
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-30

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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...	4.77	13.1	ng	500578	1	6.64	766731	20.0
unknown6.41	6.41	76.9	ng	2947820	1	6.64	766731	20.0
2(3H)-Benzothiazo...	10.60	3.4	ng	152633	4	11.16	887357	20.0
Benzenesulfonamid...	11.06	3.1	ng	138790	4	11.16	887357	20.0
Diphenyl sulfone	11.72	3.4	ng	149497	4	11.16	887357	20.0
unknown12.48	12.48	2.3	ng	67976	5	13.80	580389	20.0
Phenol, 4,4'-(1-m...	12.64	2.1	ng	62014	5	13.80	580389	20.0
Ethanol, 2-butoxy...	13.32	2.3	ng	65637	5	13.80	580389	20.0