

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032416\
 Data File : BF085729.D
 Acq On : 24 Mar 2016 22:33
 Operator : UM/SJ
 Sample : H1864-12
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PZ-6

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-BF032416.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	4.996	234	237	249	rBV	70889	113845	4.23%	0.536%
2	5.419	272	274	276	rBV	820019	951621	35.36%	4.479%
3	6.447	363	364	374	rBV2	450127	603090	22.41%	2.839%
4	6.585	374	376	379	rBV	1722105	1717877	63.83%	8.086%
5	6.825	395	397	399	rBV	654785	609471	22.65%	2.869%
6	6.973	408	410	413	rVB	1357599	1646855	61.19%	7.752%
7	7.385	444	446	449	rBV	1223380	1327570	49.33%	6.249%
8	7.636	466	468	471	rBV3	22482	44901	1.67%	0.211%
9	7.865	482	488	491	rBV3	12245	33797	1.26%	0.159%
10	8.013	498	501	507	rVB3	46626	93583	3.48%	0.441%
11	8.105	507	509	512	rBV	856988	834587	31.01%	3.928%
12	8.230	518	520	522	rBV2	18118	33821	1.26%	0.159%
13	8.299	522	526	530	rVB5	28361	87276	3.24%	0.411%
14	8.356	530	531	536	rVB3	11585	28373	1.05%	0.134%
15	8.436	536	538	539	rBV	23041	28659	1.06%	0.135%
16	8.493	539	543	546	rBV3	68176	102367	3.80%	0.482%
17	8.585	549	551	553	rVB2	37031	55142	2.05%	0.260%
18	8.642	553	556	558	rBV	62000	74287	2.76%	0.350%
19	8.756	562	566	567	rBV2	23174	56353	2.09%	0.265%
20	8.790	567	569	571	rBV3	18412	46502	1.73%	0.219%
21	8.825	571	572	575	rBV2	32956	56096	2.08%	0.264%
22	8.882	575	577	579	rVB2	25529	45374	1.69%	0.214%
23	8.939	579	582	583	rBV3	23015	36201	1.35%	0.170%
24	8.962	583	584	587	rVB2	72359	75749	2.81%	0.357%
25	9.065	589	593	594	rBV3	47264	99691	3.70%	0.469%
26	9.099	594	596	598	rVB2	46570	42337	1.57%	0.199%
27	9.145	598	600	601	rBV	62538	55792	2.07%	0.263%
28	9.191	601	604	606	rBV	2350751	2691249	100.00%	12.668%
29	9.293	609	613	616	rBV5	45049	109812	4.08%	0.517%
30	9.351	616	618	620	rBV3	38138	66194	2.46%	0.312%
31	9.431	624	625	628	rVB2	71514	90987	3.38%	0.428%
32	9.488	628	630	632	rBV2	65459	133730	4.97%	0.629%
33	9.682	644	647	649	rBV3	73051	152183	5.65%	0.716%
34	9.796	654	657	659	rVV4	59175	114571	4.26%	0.539%

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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 >
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35	9.865	660	663	665 rVV	912513	1047833	38.93%	4.932%
36	9.922	665	668	670 rVV3	54488	101915	3.79%	0.480%
37	10.013	674	676	679 rVV3	42014	69627	2.59%	0.328%
38	10.071	679	681	684 rVB2	31714	55989	2.08%	0.264%
39	10.116	684	685	687 rBV	89191	115611	4.30%	0.544%
40	10.208	691	693	696 rVV2	123075	171425	6.37%	0.807%
41	10.276	696	699	702 rVB4	44973	107574	4.00%	0.506%
42	10.413	710	711	713 rBV	78785	83664	3.11%	0.394%
43	10.448	713	714	715 rBV	37365	30846	1.15%	0.145%
44	10.539	720	722	725 rVB4	53622	62420	2.32%	0.294%
45	10.596	725	727	729 rVB2	36517	41560	1.54%	0.196%
46	10.653	729	732	734 rBV	1565582	1748335	64.96%	8.230%
47	10.768	740	742	744 rVB2	35758	44995	1.67%	0.212%
48	11.065	766	768	769 rBV2	25458	35274	1.31%	0.166%
49	11.214	777	781	783 rBV4	40476	68402	2.54%	0.322%
50	11.339	790	792	795 rVB	900887	952327	35.39%	4.483%
51	11.636	816	818	821 rVB	31763	41978	1.56%	0.198%
52	11.876	837	839	843 rVB3	59457	75684	2.81%	0.356%
53	12.654	906	907	914 rVB3	39303	69687	2.59%	0.328%
54	12.928	928	931	933 rBV	2833457	2588663	96.19%	12.185%
55	13.511	980	982	985 rVB	100935	123062	4.57%	0.579%
56	13.980	1020	1023	1025 rBV	725914	802358	29.81%	3.777%
57	15.397	1144	1147	1152 rBV	409260	545548	20.27%	2.568%

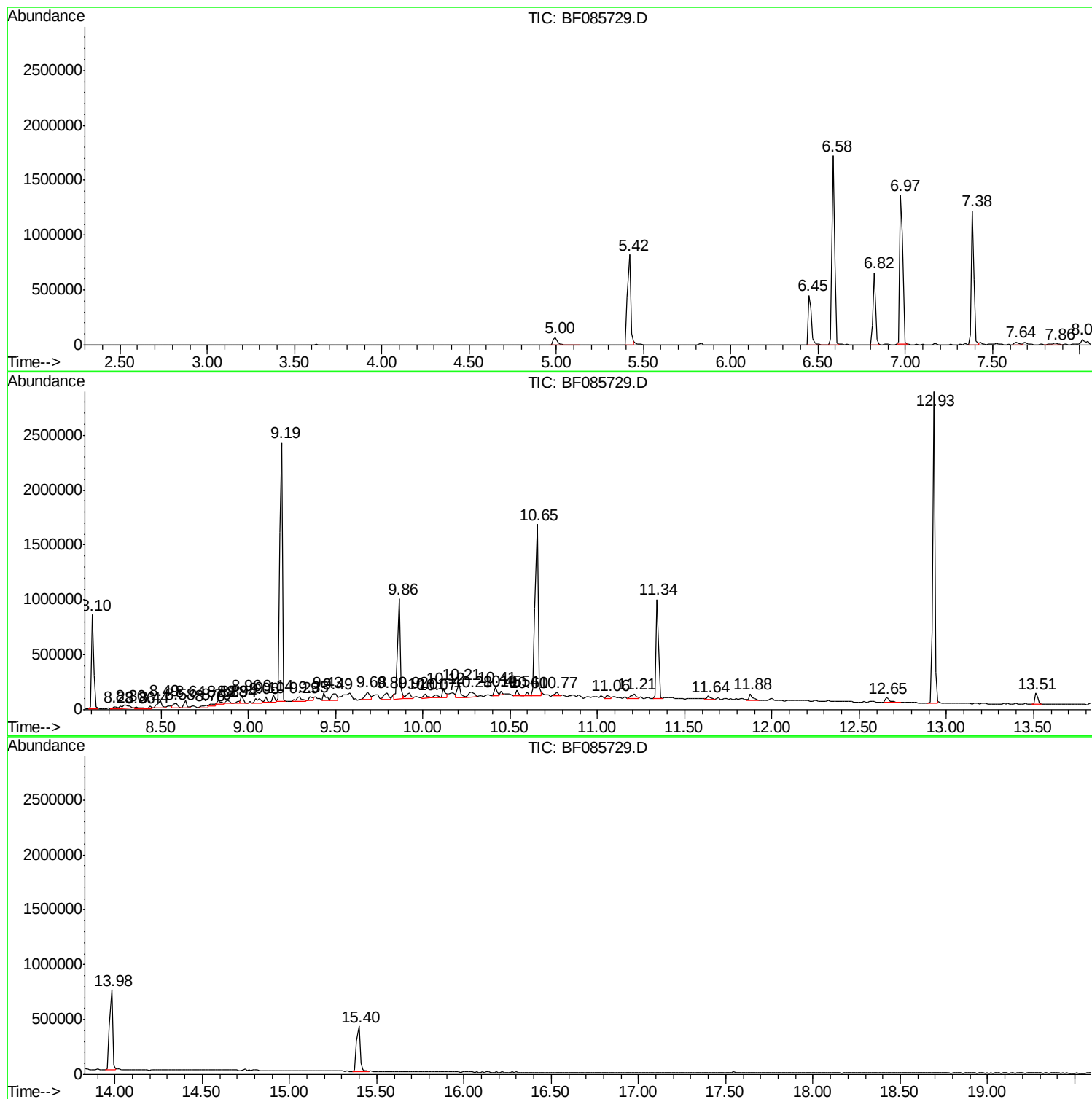
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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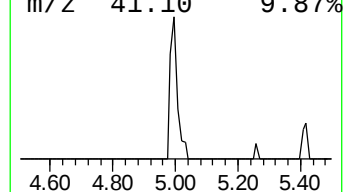
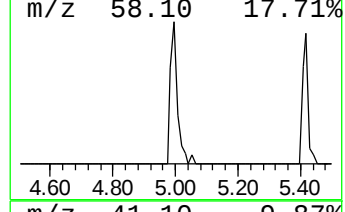
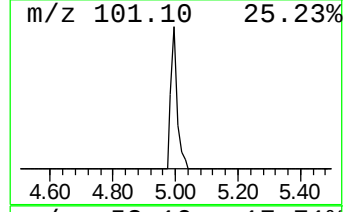
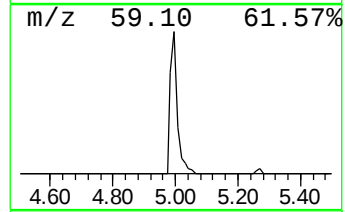
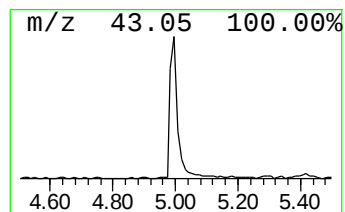
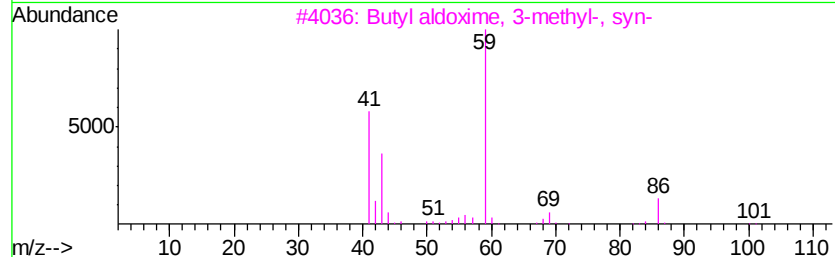
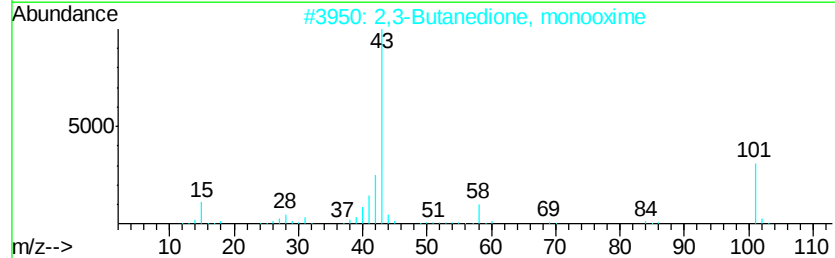
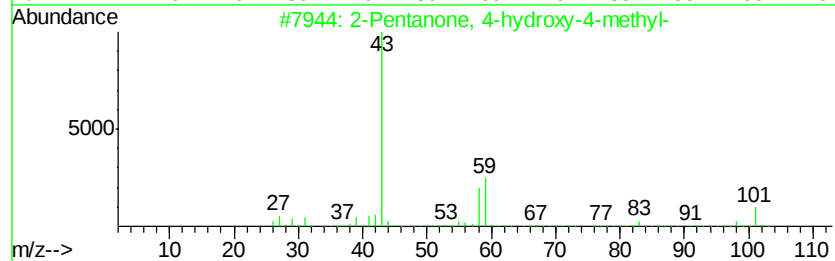
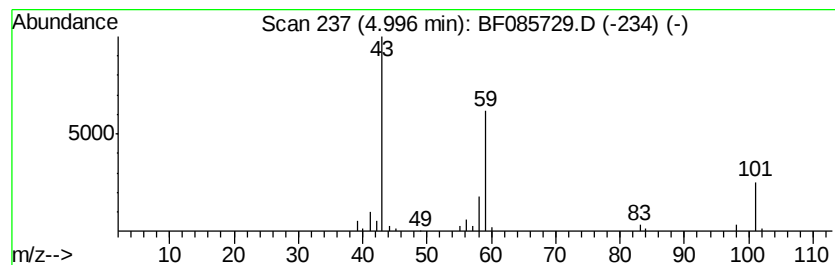
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.00	3.74 ng	113845	1,4-Dichlorobenzene-d4	6.82

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56	
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38	
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25	
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23	
5	Acetone	58	C3H6O	000067-64-1	10	



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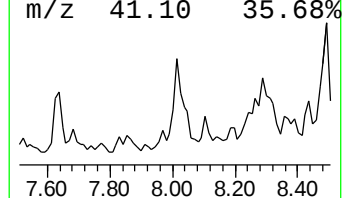
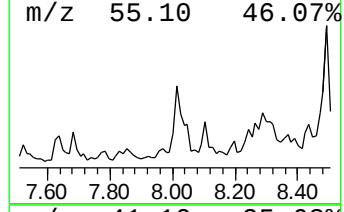
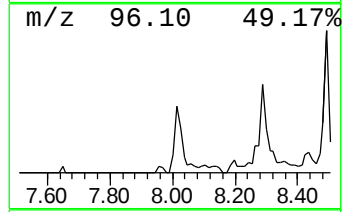
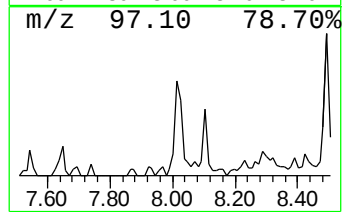
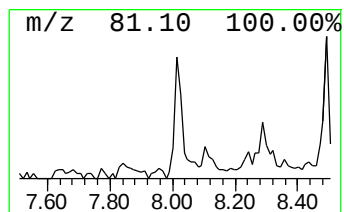
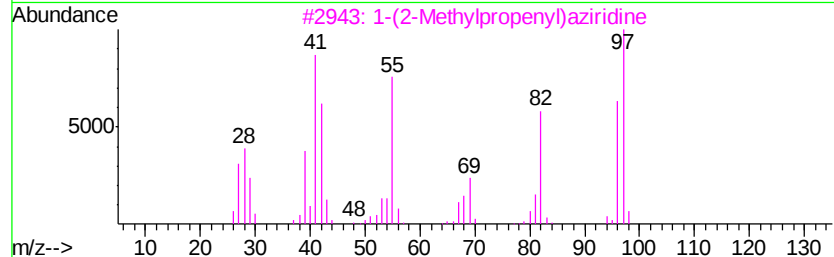
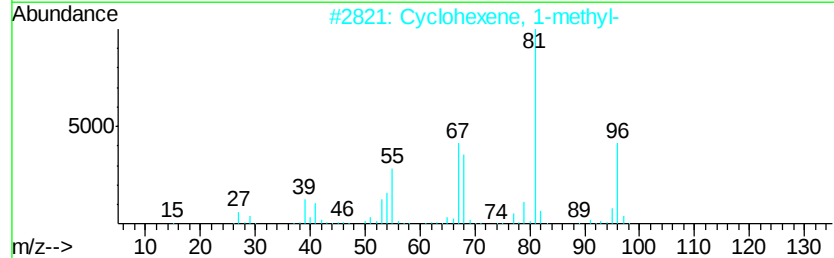
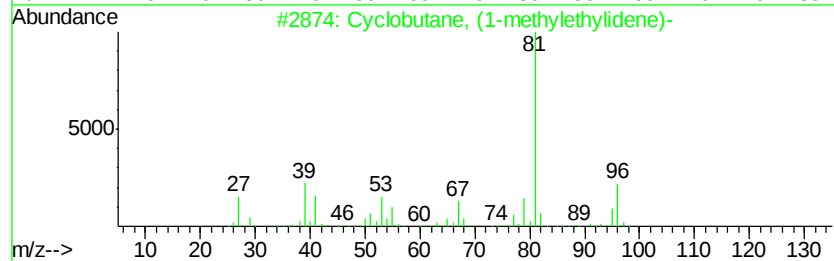
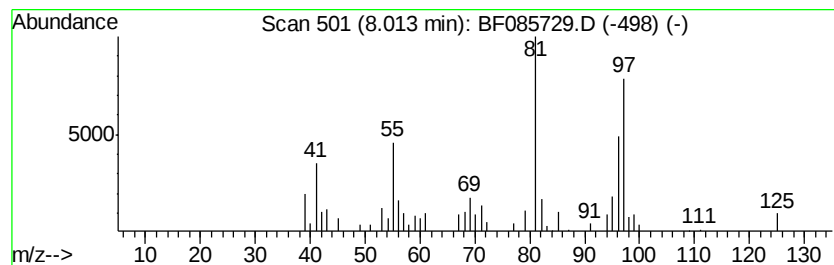
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown8.01 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.01	2.24 ng	93583	Naphthalene-d8	8.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclobutane, (1-methylethylidene)-	96	C7H12	001528-22-9	43
2		Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	38
3		1-(2-Methylpropenyl)aziridine	97	C6H11N	080839-93-6	38
4		Cyclohexane, methylene-	96	C7H12	001192-37-6	38
5		6-Methyl-bicyclo[4.2.0]octan-7-one	138	C9H14O	1000193-87-2	37



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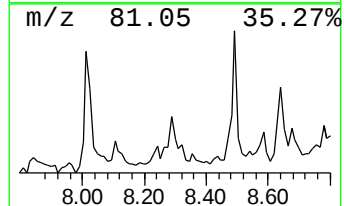
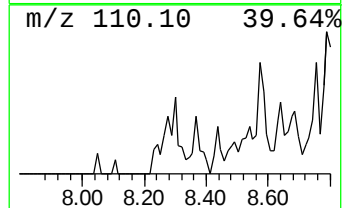
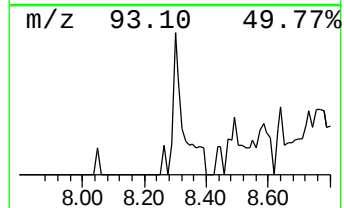
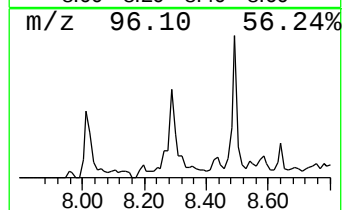
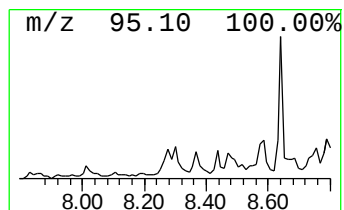
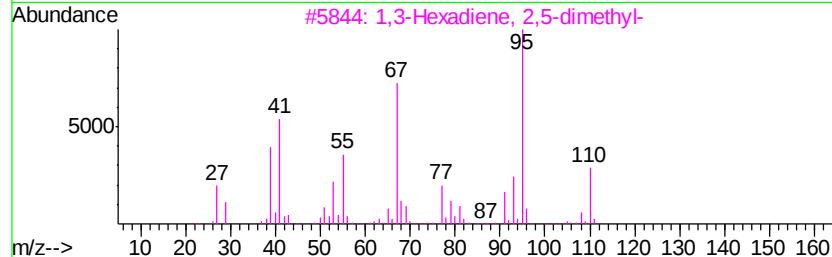
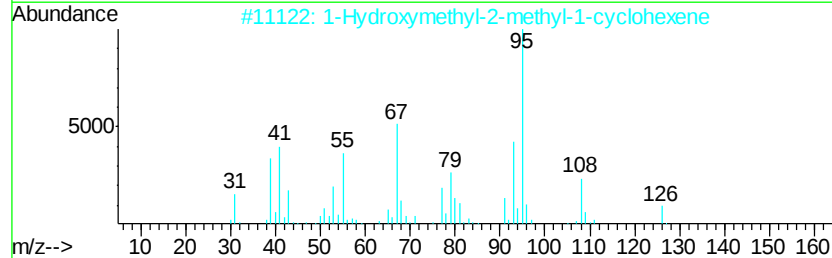
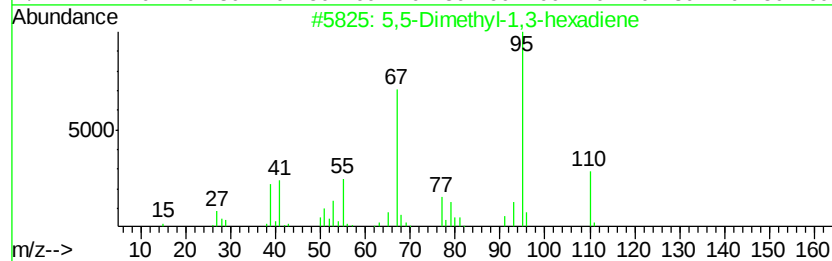
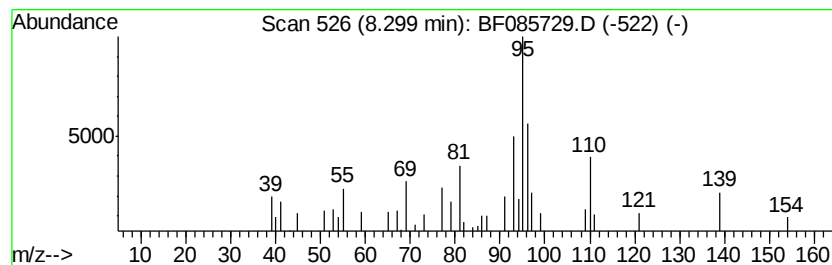
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown8.30 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.30	2.09 ng	87276	Naphthalene-d8	8.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	38
2		1-Hydroxymethyl-2-methyl-1-cyclo...	126	C8H14O	029474-11-1	32
3		1,3-Hexadiene, 2,5-dimethyl-	110	C8H14	029253-64-3	32
4		Furan, 2-ethyl-5-methyl-	110	C7H10O	001703-52-2	32
5		2-Pentynal semicarbazone	139	C6H9N3O	117785-63-4	32



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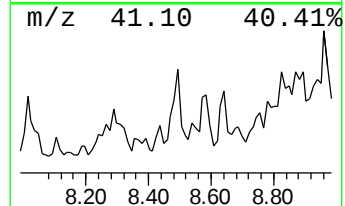
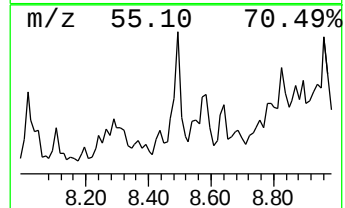
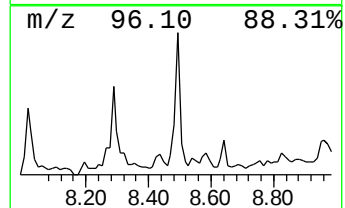
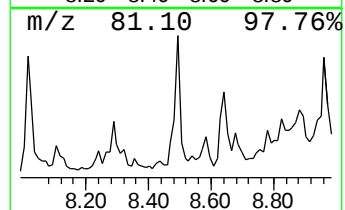
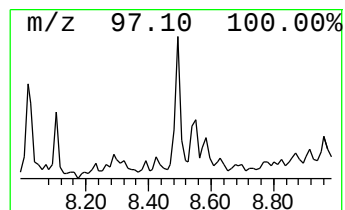
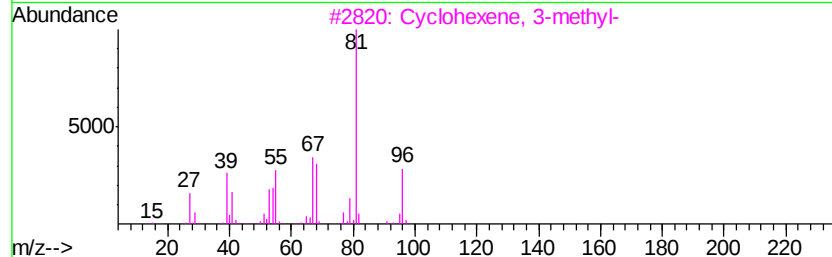
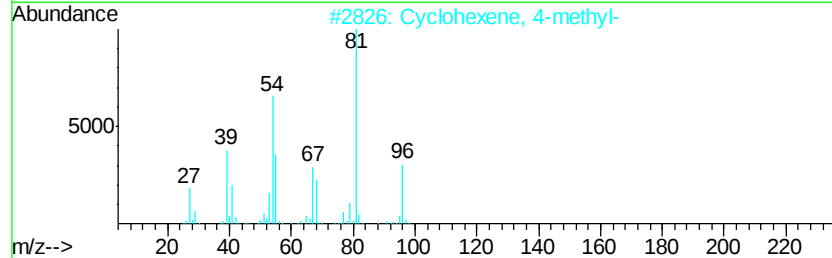
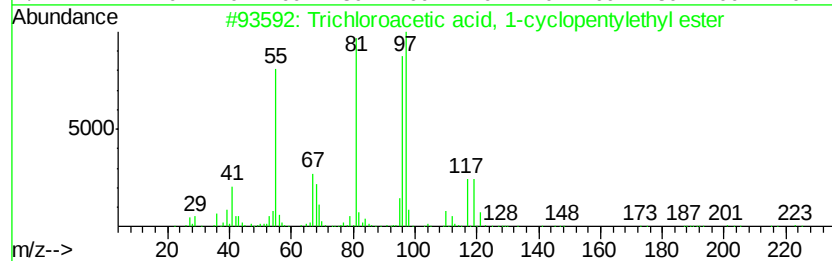
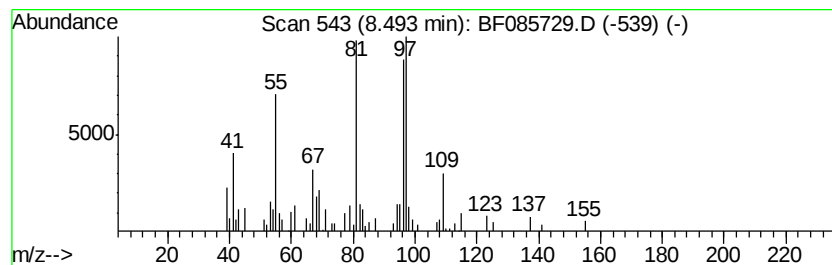
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Trichloroacetic acid, 1-cyc... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
8.49	2.45 ng	102367	Naphthalene-d8	8.10		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trichloroacetic acid, 1-cyclopent...	258	C9H13Cl3O2	1000282-57-1	72
2		Cyclohexene, 4-methyl-	96	C7H12	000591-47-9	46
3		Cyclohexene, 3-methyl-	96	C7H12	000591-48-0	46
4		Furan, 2-ethyl-	96	C6H8O	003208-16-0	43
5		2,4-Hexadiene, 2-methyl-	96	C7H12	028823-41-8	43



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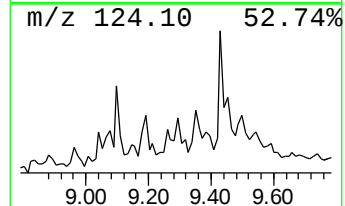
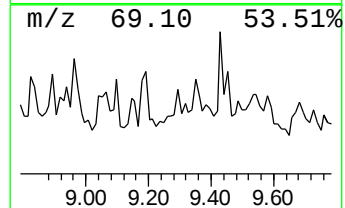
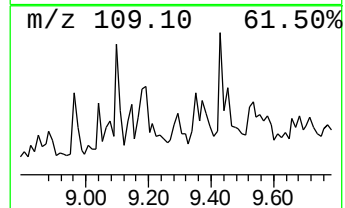
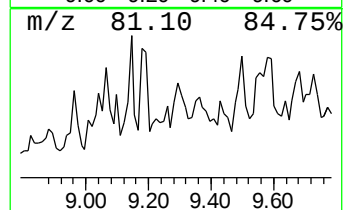
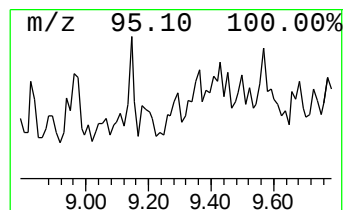
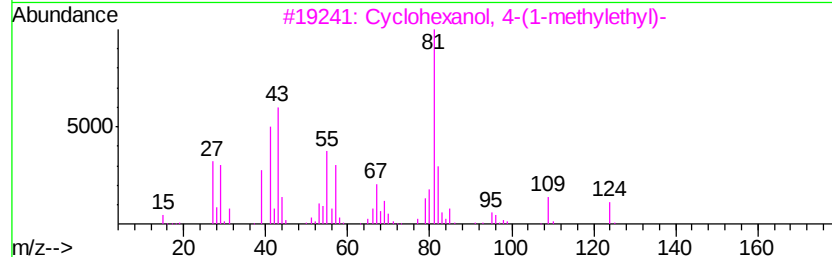
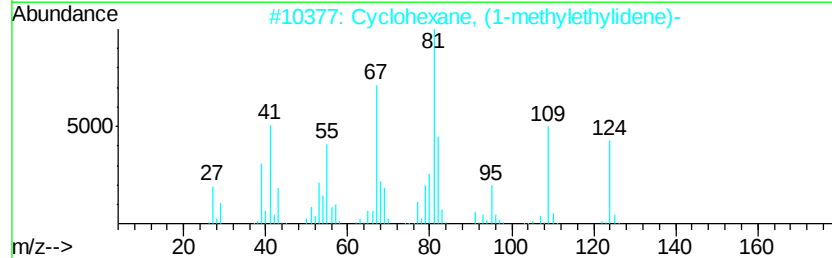
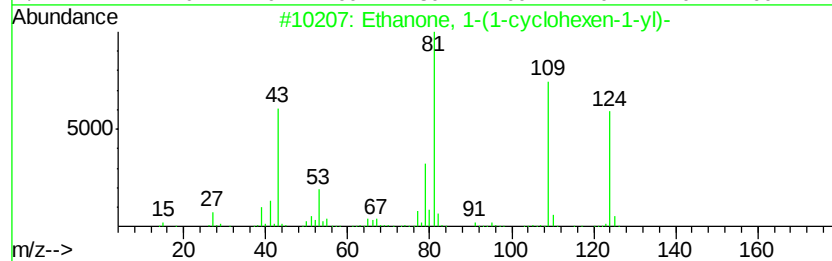
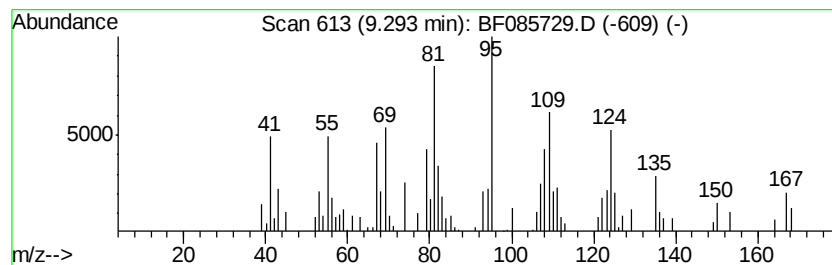
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown9.29 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.29	2.10 ng	109812	Acenaphthene-d10	9.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanone, 1-(1-cyclohexen-1-yl)-	124	C8H12O	000932-66-1	38
2		Cyclohexane, (1-methylethylidene)-	124	C9H16	005749-72-4	35
3		Cyclohexanol, 4-(1-methylethyl)-	142	C9H18O	004621-04-9	22
4		Bicyclo[2.2.1]heptane, 1,3,3-tri...	138	C10H18	006248-88-0	22
5		Iridomyrmecin	168	C10H16O2	000485-43-8	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032416\
Data File : BF085729.D
Acq On : 24 Mar 2016 22:33
Operator : UM/SJ
Sample : H1864-12
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
PZ-6

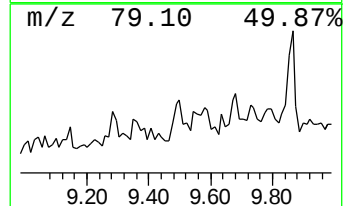
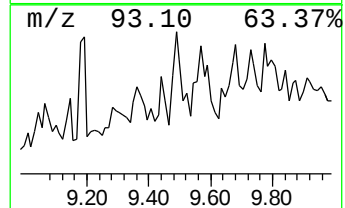
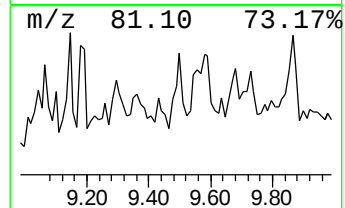
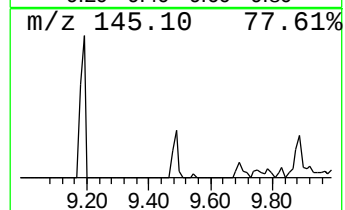
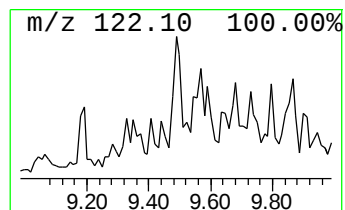
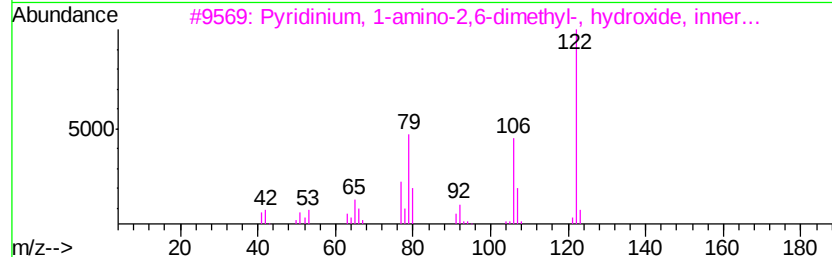
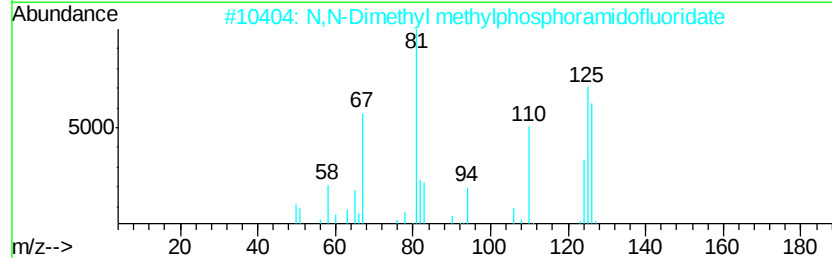
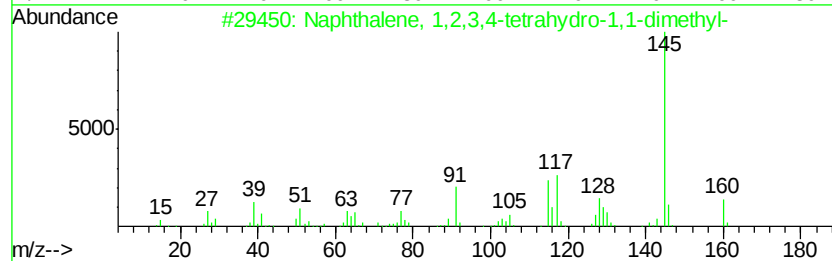
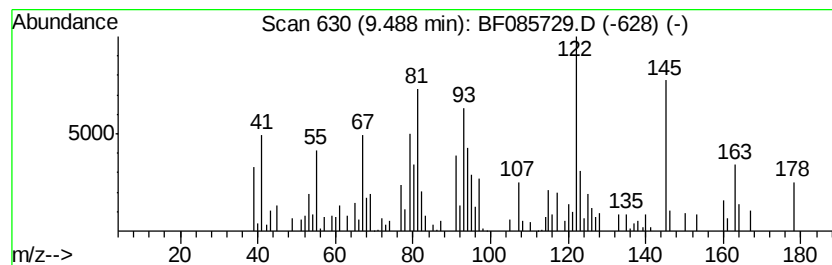
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown9.49 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.49	2.55 ng	133730	Acenaphthene-d10	9.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	001985-59-7	25
2		N,N-Dimethyl methylphosphoramido...	125	C3H9FNOP	000661-60-9	25
3		Pyridinium, 1-amino-2,6-dimethyl...	122	C7H10N2	051135-76-3	25
4		2-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	000432-24-6	25
5		2-Pyridinamine, 4,6-dimethyl-	122	C7H10N2	005407-87-4	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032416\
Data File : BF085729.D
Acq On : 24 Mar 2016 22:33
Operator : UM/SJ
Sample : H1864-12
Misc :
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Instrument :
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ClientSampleId :
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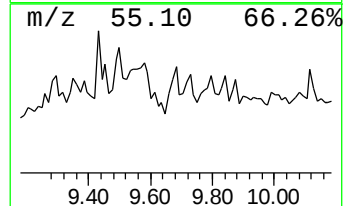
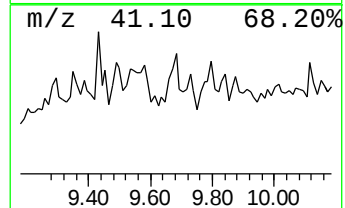
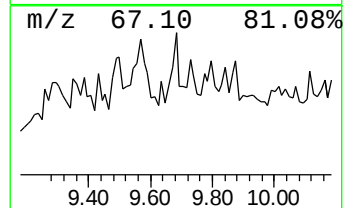
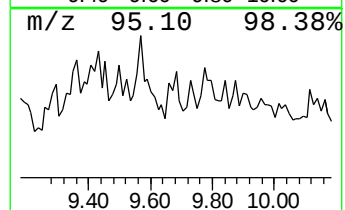
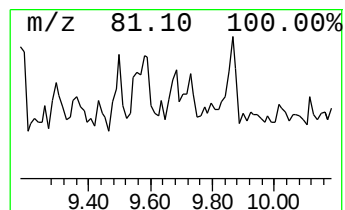
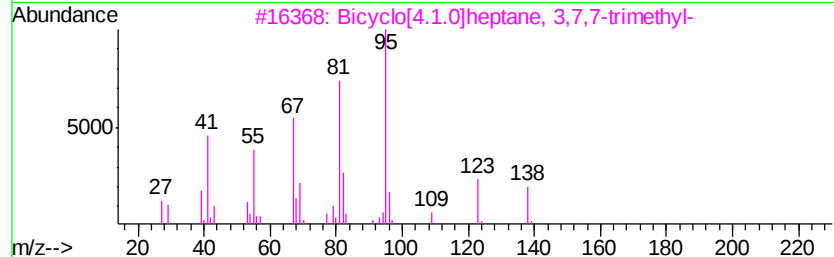
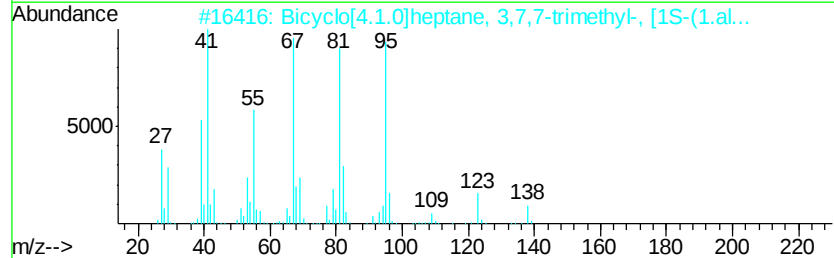
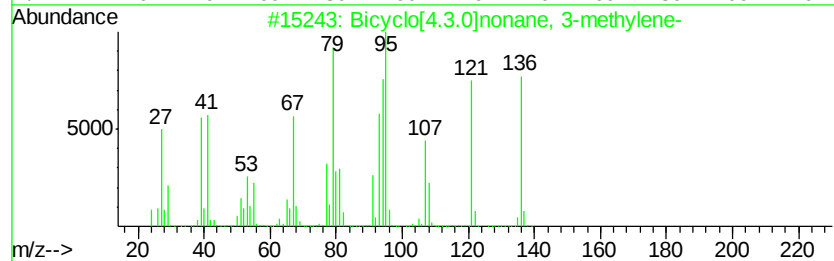
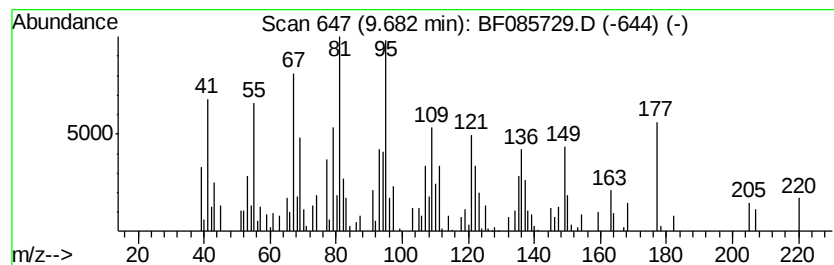
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Bicyclo[4.3.0]nonane, 3-met... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.68	2.90 ng	152183	Acenaphthene-d10	9.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[4.3.0]nonane, 3-methylene-	136	C10H16	1000152-00-6	64
2		Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	006069-97-2	50
3		Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	000554-59-6	45
4		Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	000473-19-8	41
5		Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-41-8	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032416\
Data File : BF085729.D
Acq On : 24 Mar 2016 22:33
Operator : UM/SJ
Sample : H1864-12
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PZ-6

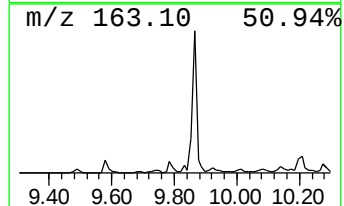
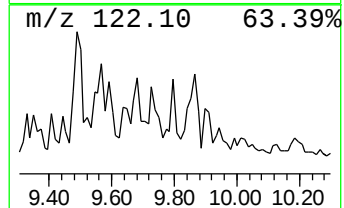
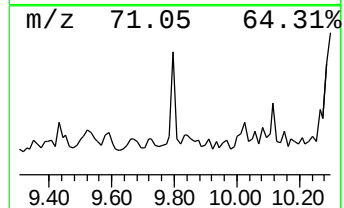
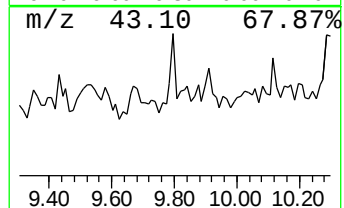
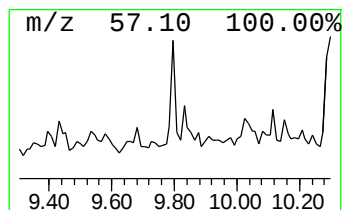
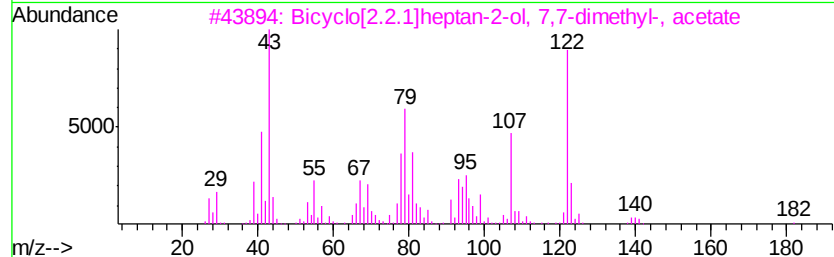
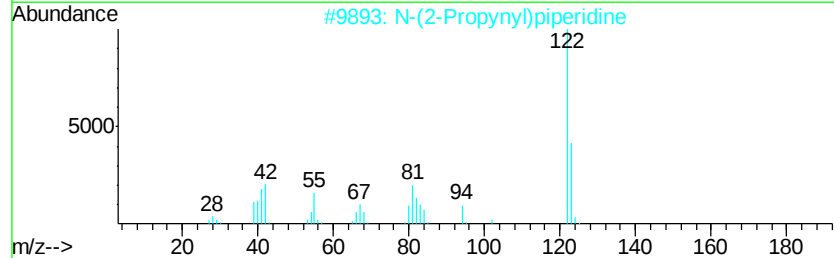
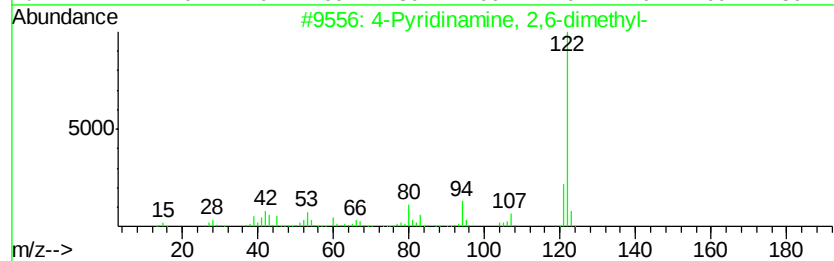
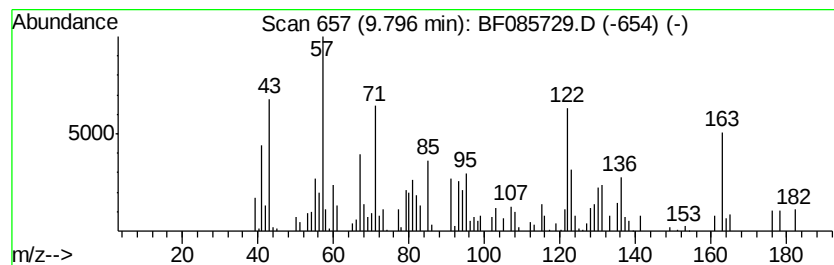
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown9.80 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.80	2.19 ng	114571	Acenaphthene-d10	9.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Pyridinamine, 2,6-dimethyl-	122	C7H10N2	003512-80-9	22
2			N-(2-Propynyl)piperidine	123	C8H13N	005799-75-7	18
3			Bicyclo[2.2.1]heptan-2-ol, 7,7-d...	182	C11H18O2	062555-02-6	14
4			2-Propenal, 3-(2,6,6-trimethyl-1...	178	C12H18O	004951-40-0	11
5			s-Triazolo[4,3-a]pyrazine, 3-ami...	163	C7H9N5	019855-02-8	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032416\
Data File : BF085729.D
Acq On : 24 Mar 2016 22:33
Operator : UM/SJ
Sample : H1864-12
Misc :
ALS Vial : 16 Sample Multiplier: 1

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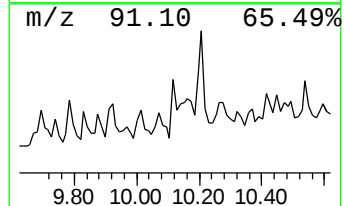
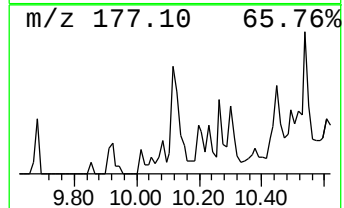
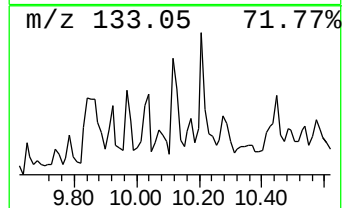
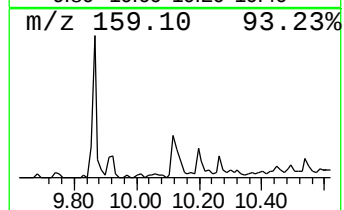
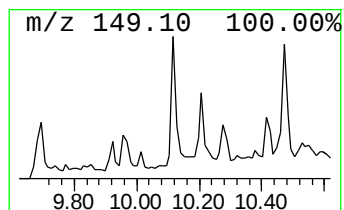
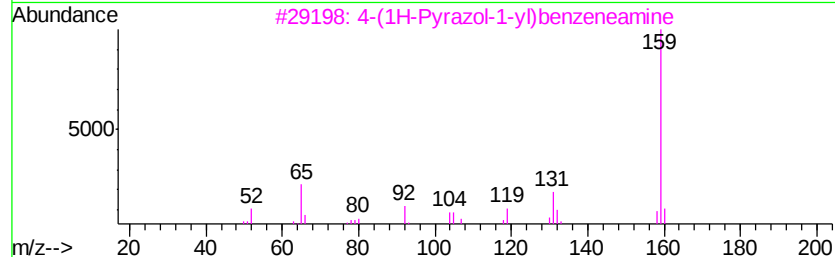
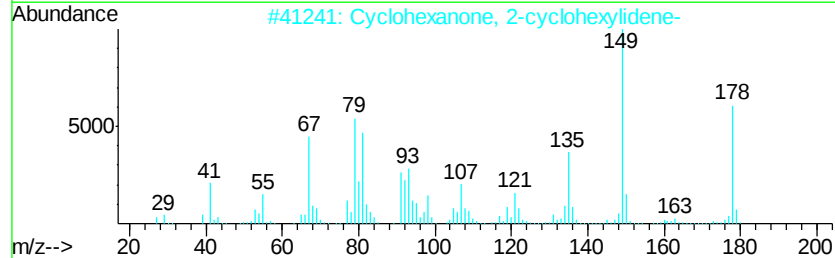
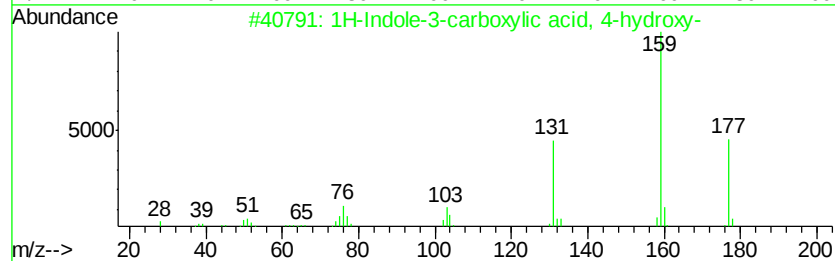
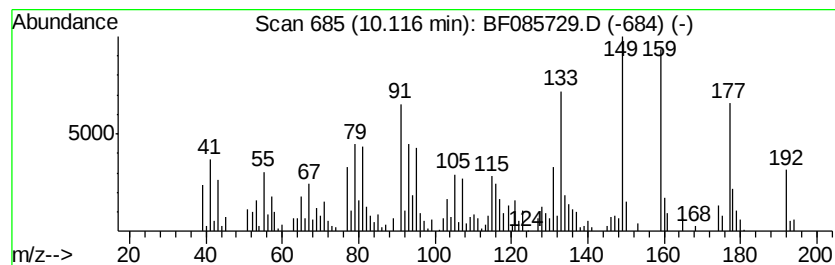
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown10.12 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.12	2.21 ng	115611	Acenaphthene-d10	9.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Indole-3-carboxylic acid, 4-h...	177	C9H7NO3	024370-76-1	30
2		Cyclohexanone, 2-cyclohexylidene-	178	C12H18O	001011-12-7	25
3		4-(1H-Pyrazol-1-yl)benzeneamine	159	C9H9N3	017635-45-9	25
4		4-Hydroxy-4-methyl-4H-naphthalen...	174	C11H10O2	042860-82-2	25
5		Benzeneacetaldehyde, 2-methoxy-....	178	C11H14O2	053155-90-1	15



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032416\
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Acq On : 24 Mar 2016 22:33
Operator : UM/SJ
Sample : H1864-12
Misc :
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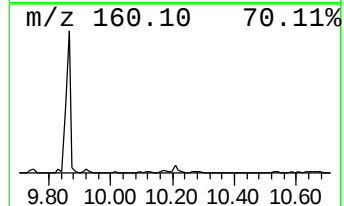
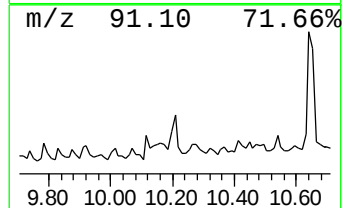
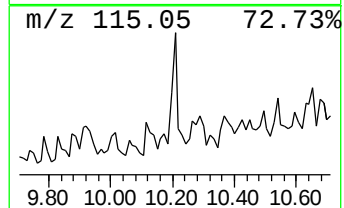
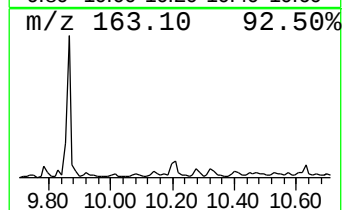
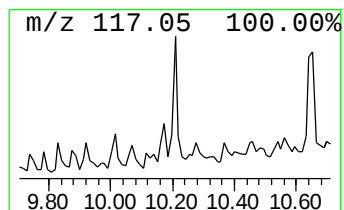
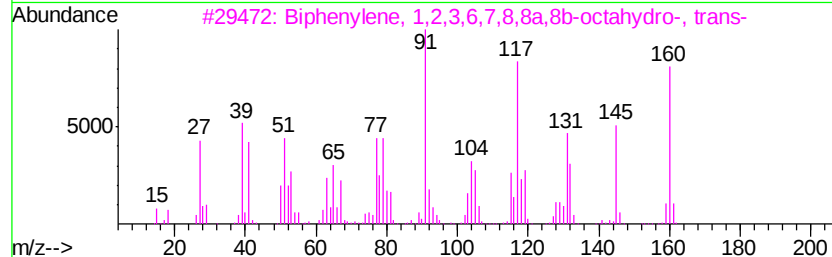
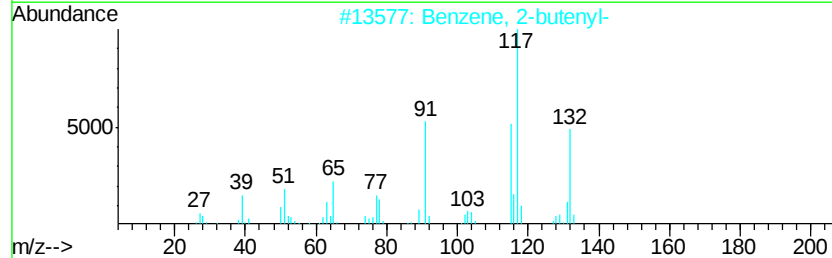
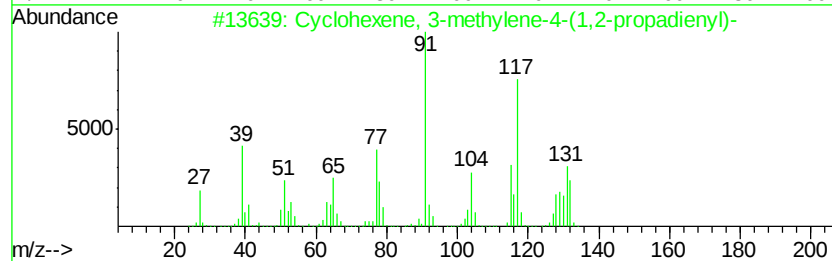
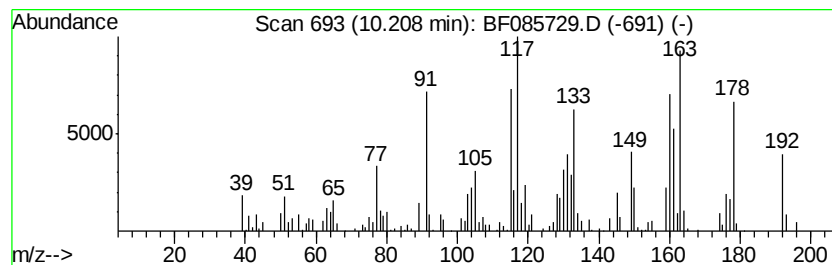
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown10.21 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.21	3.27 ng	171425	Acenaphthene-d10	9.86
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexene, 3-methylene-4-(1,2-...	132 C10H12	068377-81-1 25
2		Benzene, 2-butenyl-	132 C10H12	001560-06-1 25
3		Biphenylene, 1,2,3,6,7,8,8a,8b-o...	160 C12H16	028229-15-4 15
4		3,8-Dihydroxy-3,4-dihydronaphtha...	178 C10H10O3	059796-04-2 15
5		2-Propenoic acid, 3-(4-methoxyph...	192 C11H12O3	003901-07-3 15



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032416\
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Misc :
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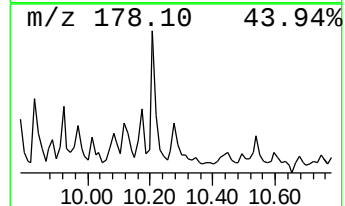
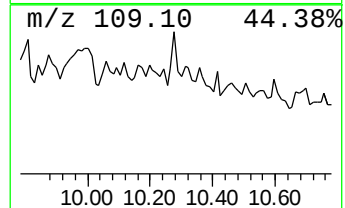
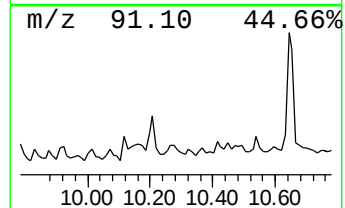
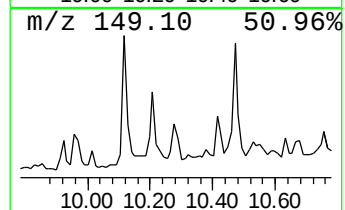
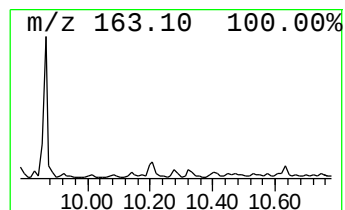
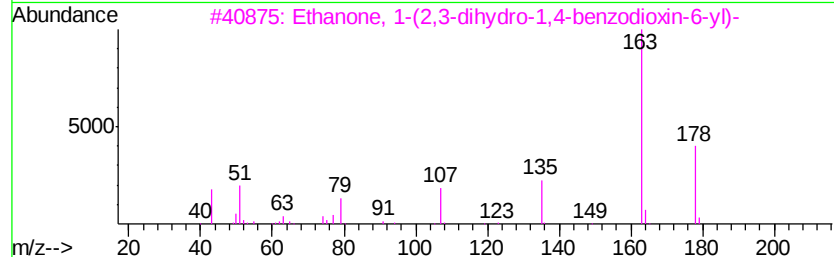
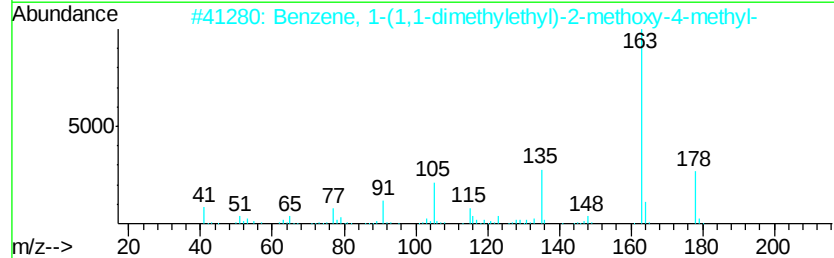
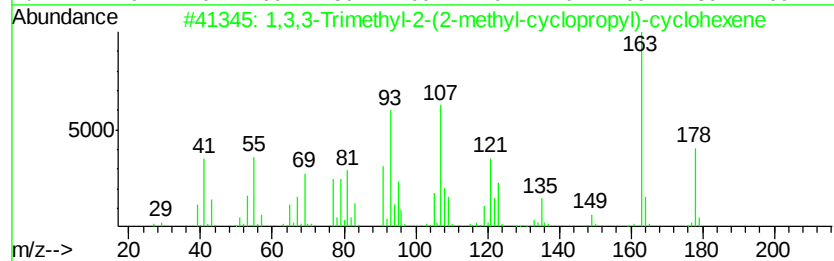
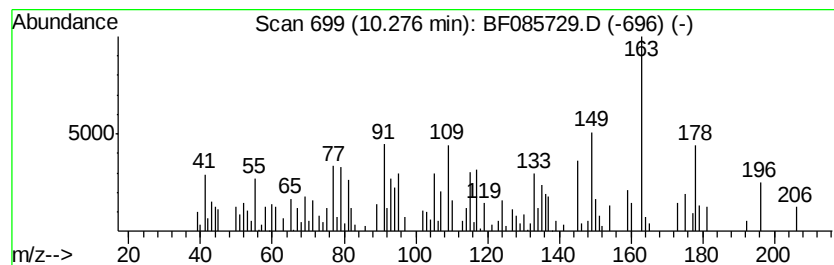
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown10.28 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.28	2.05 ng	107574	Acenaphthene-d10	9.86
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1,3,3-Trimethyl-2-(2-methyl-cycl...	178 C13H22	285129-06-8	27
2	Benzene, 1-(1,1-dimethylethyl)-2...	178 C12H180	000088-40-4	27
3	Ethanone, 1-(2,3-dihydro-1,4-ben...	178 C10H1003	002879-20-1	25
4	Methyl 2-ethylhexyl phthalate	292 C17H2404	056166-83-7	22
5	2-Propanone, 1-(3,5,5-trimethyl-...	178 C12H180	016695-73-1	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032416\
Data File : BF085729.D
Acq On : 24 Mar 2016 22:33
Operator : UM/SJ
Sample : H1864-12
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PZ-6

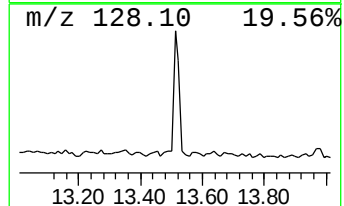
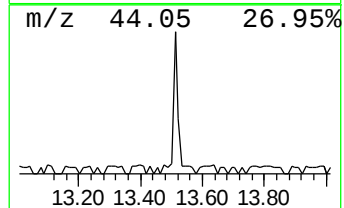
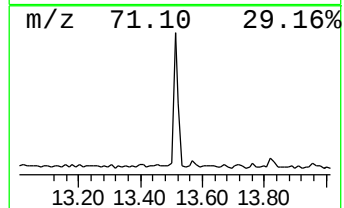
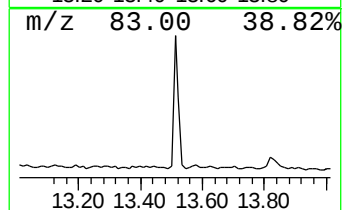
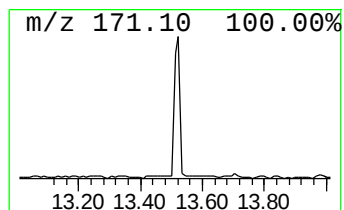
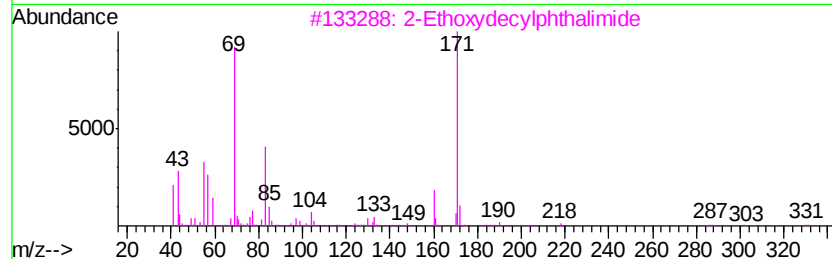
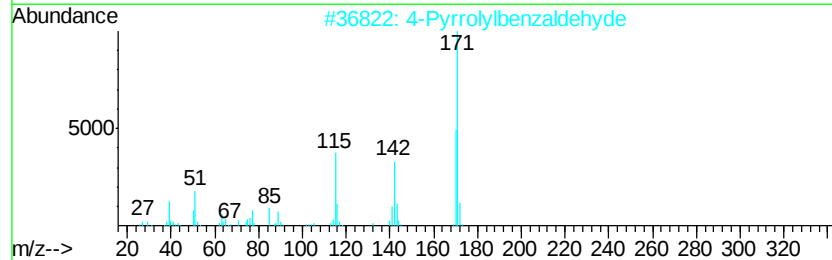
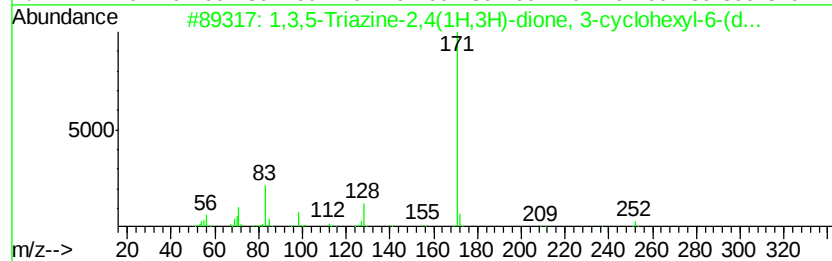
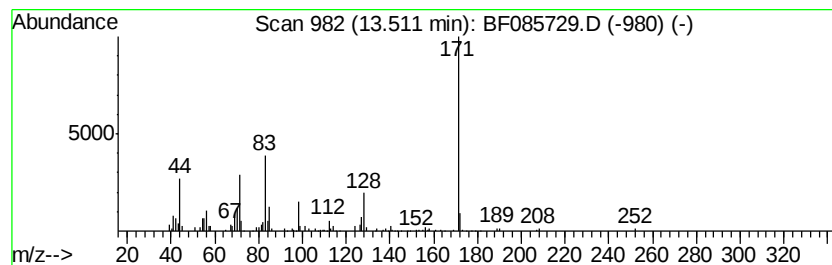
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 1,3,5-Triazine-2,4(1H,3H)-d... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.51	3.07 ng	123062	Chrysene-d12	13.98

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3,5-Triazine-2,4(1H,3H)-dione, ...	252	C12H20N4O2	051235-04-2	94
2			4-Pyrrolylbenzaldehyde	171	C11H9NO	023351-05-5	35
3			2-Ethoxydecylphthalimide	331	C20H29NO3	1000227-42-3	33
4			Benzoic acid, 2,6-difluoro-4-met...	202	C9H8F2O3	084937-82-6	32
5			3-Cyanoquinoxaline 1-oxide	171	C9H5N3O	053688-02-1	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032416\
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Sample : H1864-12
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PZ-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.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...	5.00	3.7	ng	113845	1	6.82	609471	20.0
unknown8.01	8.01	2.2	ng	93583	2	8.10	834587	20.0
unknown8.30	8.30	2.1	ng	87276	2	8.10	834587	20.0
Trichloroacetic a...	8.49	2.5	ng	102367	2	8.10	834587	20.0
unknown9.29	9.29	2.1	ng	109812	3	9.86	1047830	20.0
unknown9.49	9.49	2.5	ng	133730	3	9.86	1047830	20.0
Bicyclo[4.3.0]non...	9.68	2.9	ng	152183	3	9.86	1047830	20.0
unknown9.80	9.80	2.2	ng	114571	3	9.86	1047830	20.0
unknown10.12	10.12	2.2	ng	115611	3	9.86	1047830	20.0
unknown10.21	10.21	3.3	ng	171425	3	9.86	1047830	20.0
unknown10.28	10.28	2.0	ng	107574	3	9.86	1047830	20.0
1,3,5-Triazine-2,...	13.51	3.1	ng	123062	5	13.98	802358	20.0