

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100416\
 Data File : BF090342.D
 Acq On : 4 Oct 2016 14:18
 Operator : UM/SJ
 Sample : H4998-07
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SUP-B045-0-3

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-BF100416.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	1.850	22	23	25	rBV	918911	1238825	6.54%	1.053%
2	1.918	25	29	32	rVB	11398458	18935939	100.00%	16.088%
3	1.998	34	36	66	rVB	7011445	16319902	86.18%	13.865%
4	2.353	66	67	101	rVB2	107847	673364	3.56%	0.572%
5	5.210	315	317	321	rBV	1081143	1609935	8.50%	1.368%
6	5.621	349	353	355	rBV	6214719	7968226	42.08%	6.770%
7	6.627	438	441	443	rBV	6734874	7131185	37.66%	6.059%
8	6.776	451	454	456	rBV	8013101	7501542	39.62%	6.373%
9	7.004	472	474	477	rVB	1766665	1972981	10.42%	1.676%
10	7.164	486	488	490	rVB	5869939	5340280	28.20%	4.537%
11	7.564	520	523	526	rBV	3357332	4907179	25.91%	4.169%
12	8.296	584	587	589	rBV	3362082	2807703	14.83%	2.385%
13	8.856	634	636	638	rVB	254297	217670	1.15%	0.185%
14	9.370	679	681	684	rVV	6422533	8296197	43.81%	7.048%
15	9.496	687	692	698	rVB2	114898	257429	1.36%	0.219%
16	9.770	713	716	718	rBV	4758944	4151872	21.93%	3.527%
17	10.056	738	741	743	rVB	3852652	3212017	16.96%	2.729%
18	10.456	774	776	778	rBV	187402	285712	1.51%	0.243%
19	10.845	807	810	812	rBV	6061218	5635049	29.76%	4.788%
20	10.959	818	820	825	rVB	172440	239855	1.27%	0.204%
21	11.051	826	828	831	rVB	234575	230306	1.22%	0.196%
22	11.542	869	871	874	rBV	3055985	2900696	15.32%	2.464%
23	11.771	888	891	893	rBV	637749	566590	2.99%	0.481%
24	12.068	914	917	925	rBV2	510502	900220	4.75%	0.765%
25	12.594	961	963	965	rBV	366775	347119	1.83%	0.295%
26	12.856	983	986	992	rBV	421698	701587	3.71%	0.596%
27	13.142	1008	1011	1013	rBV	8338942	8364334	44.17%	7.106%
28	14.034	1087	1089	1095	rBV	216508	249476	1.32%	0.212%
29	14.194	1100	1103	1105	rBV	3043338	2676553	14.13%	2.274%
30	15.702	1231	1235	1238	rBV	1247387	1775410	9.38%	1.508%
31	17.017	1345	1350	1363	rVB2	56921	286995	1.52%	0.244%

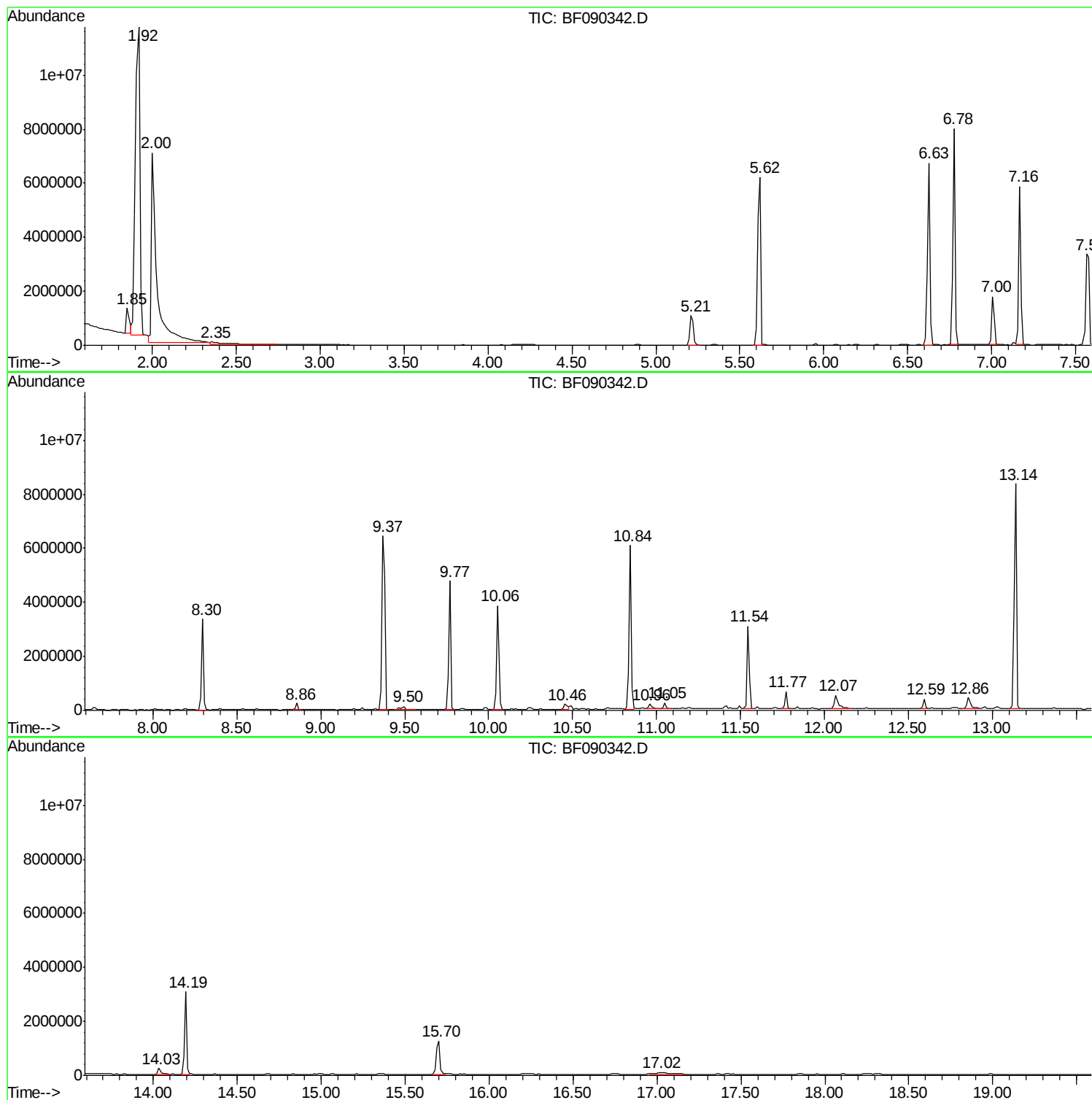
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ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleID :
SUP-B045-0-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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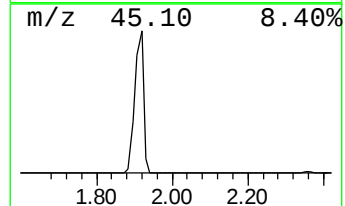
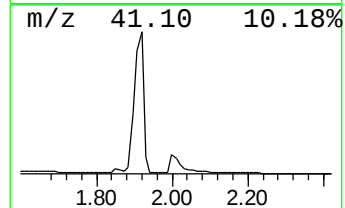
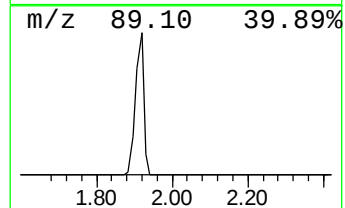
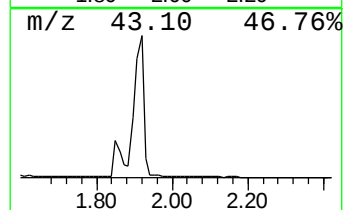
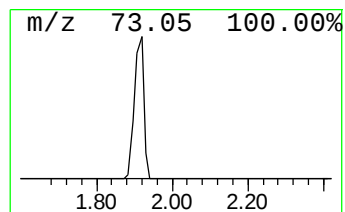
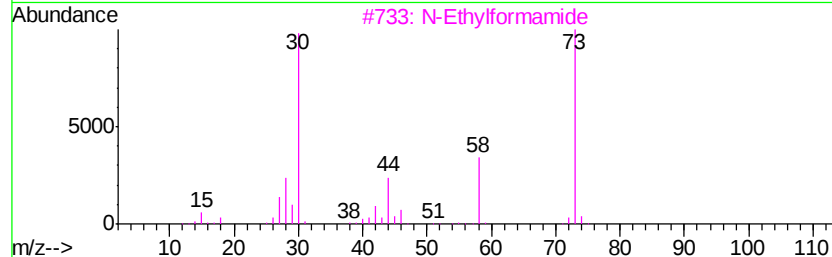
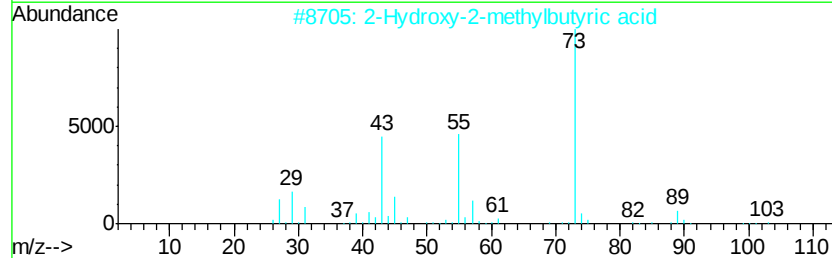
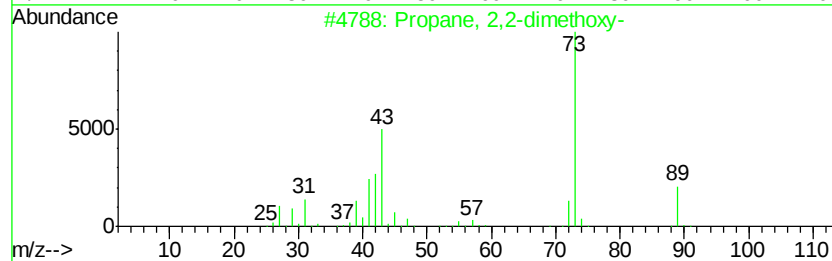
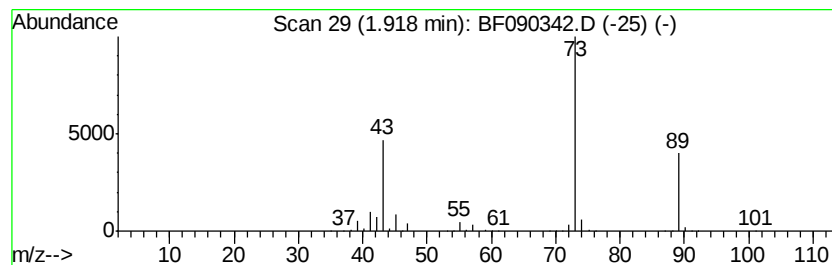
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.92	191.95 ng	18935900	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	72
2		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	23
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9



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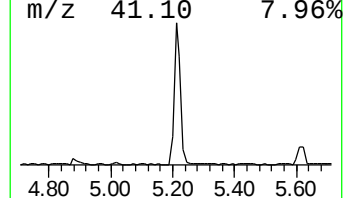
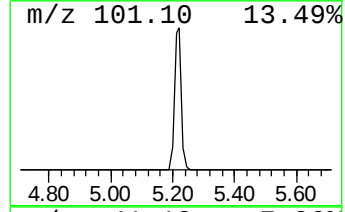
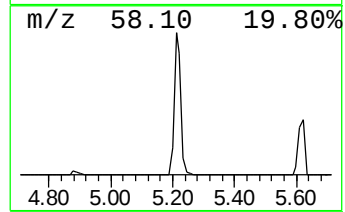
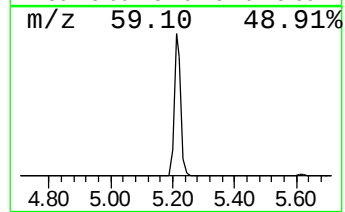
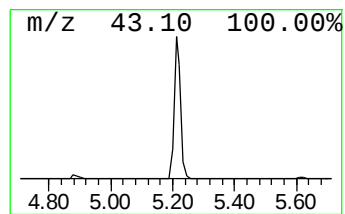
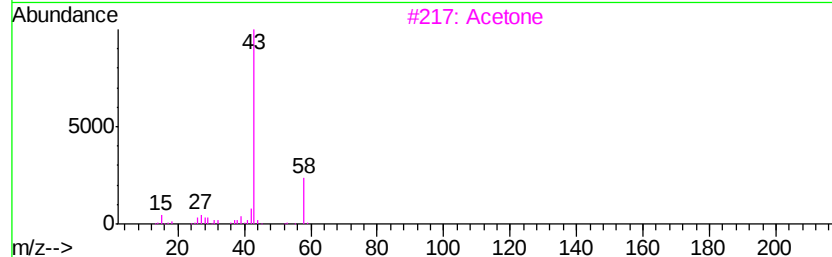
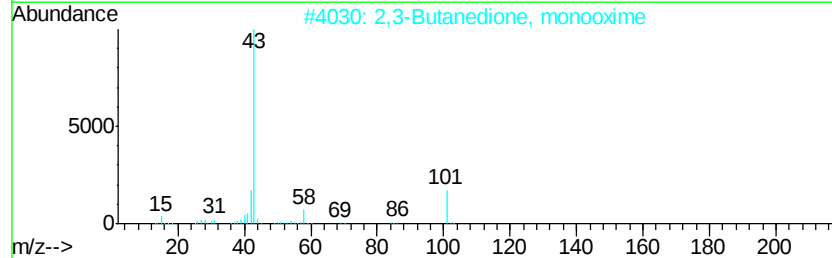
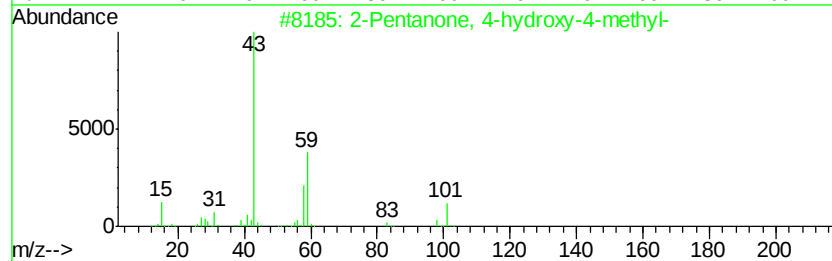
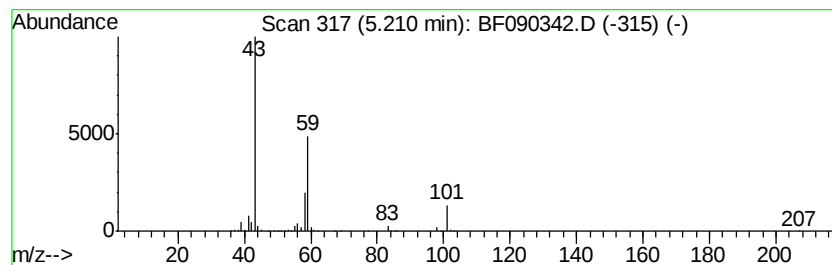
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Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	16.32 ng	1609940	1,4-Dichlorobenzene-d4	7.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	83	
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12	
3	Acetone	58	C3H6O	000067-64-1	9	
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9	
5	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	7	



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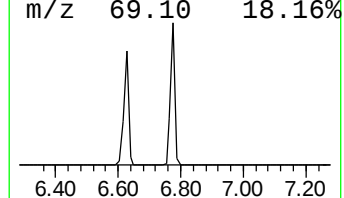
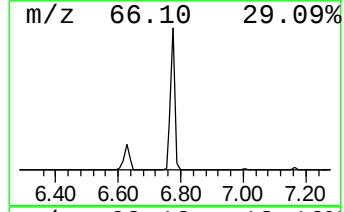
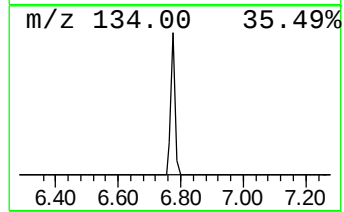
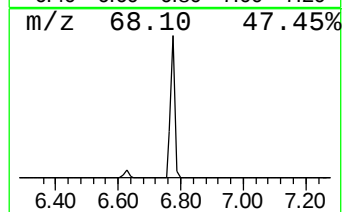
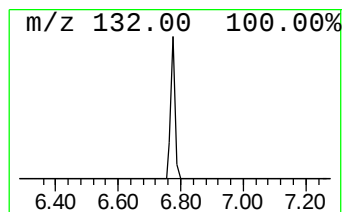
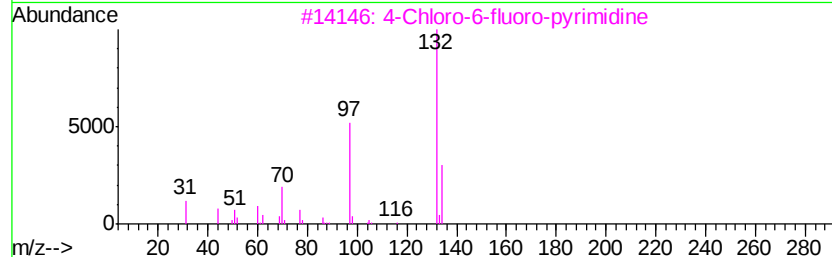
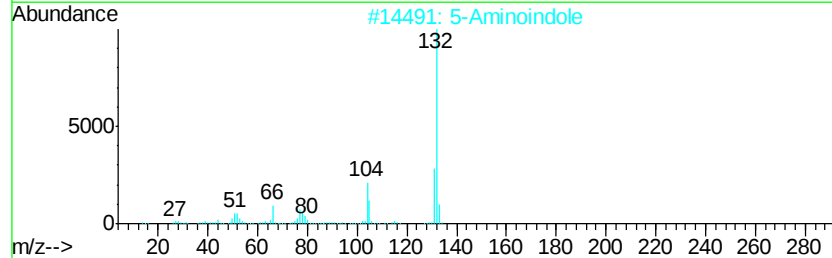
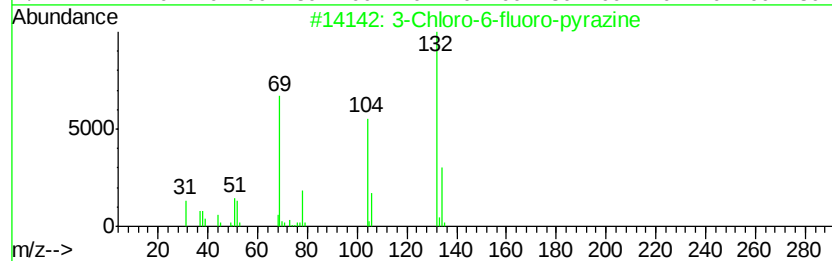
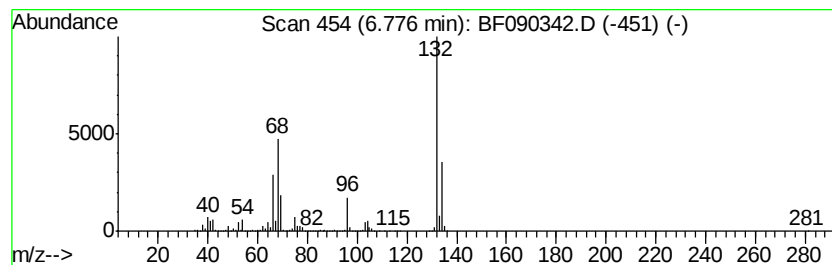
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown6.78 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	76.04 ng	7501540	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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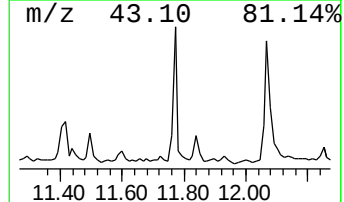
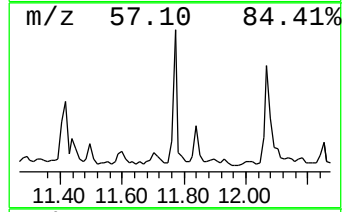
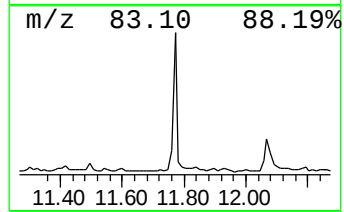
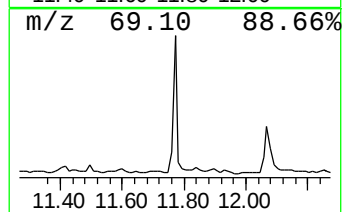
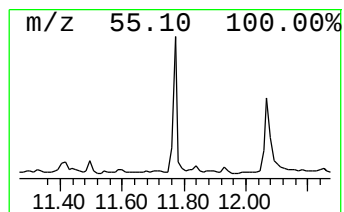
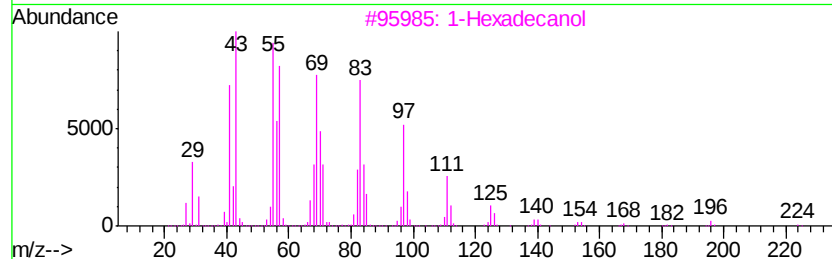
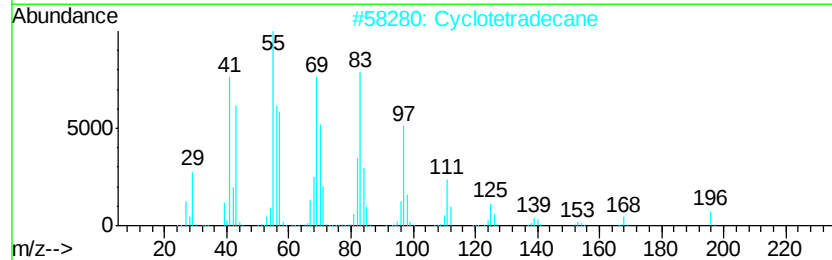
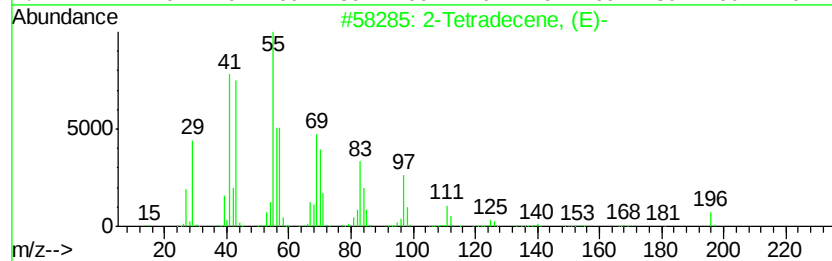
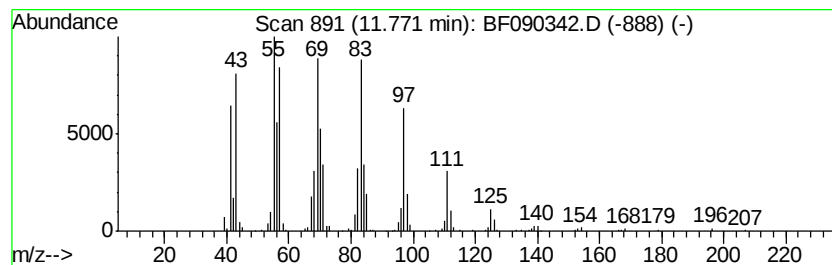
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 8 2-Tetradecene, (E)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.		
11.77	3.91 ng	566590	Phenanthrene-d10		11.54		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Tetradecene, (E)-	196	C14H28	035953-54-9	97
2			Cyclotetradecane	196	C14H28	000295-17-0	96
3			1-Hexadecanol	242	C16H34O	036653-82-4	94
4			Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	93
5			n-Tridecan-1-ol	200	C13H28O	000112-70-9	91



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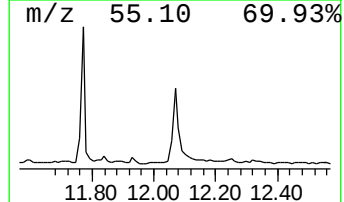
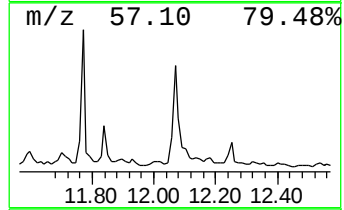
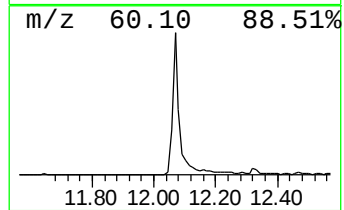
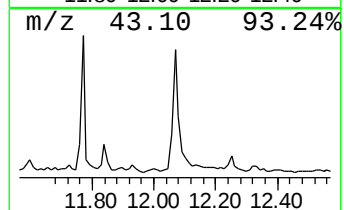
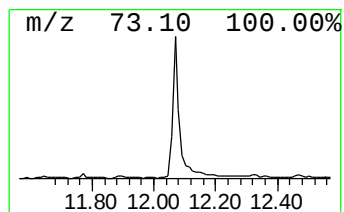
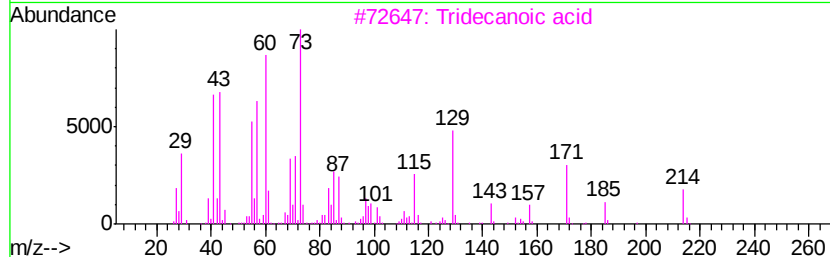
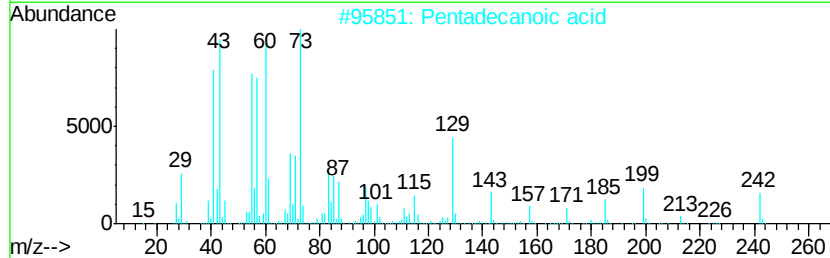
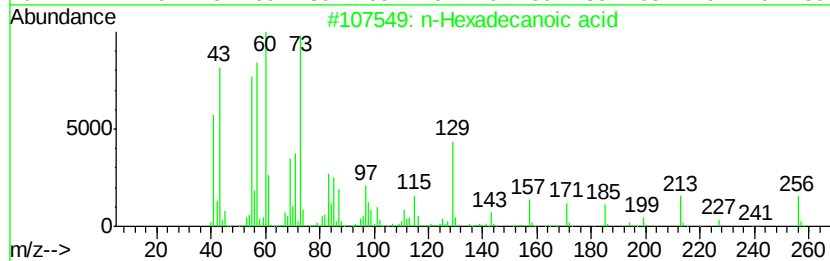
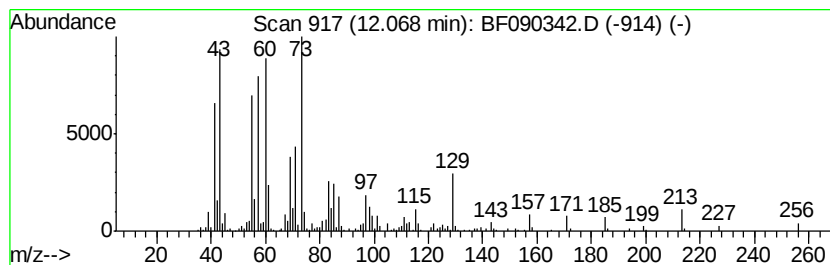
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 9 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.07	6.21 ng	900220	Phenanthrene-d10	11.54

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		Tridecanoic acid	214	C13H26O2	000638-53-9	86
4		Undecanoic acid	186	C11H22O2	000112-37-8	86
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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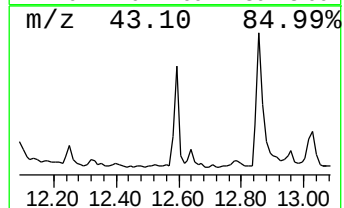
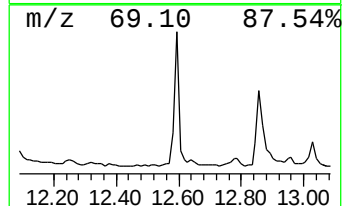
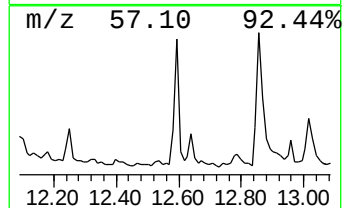
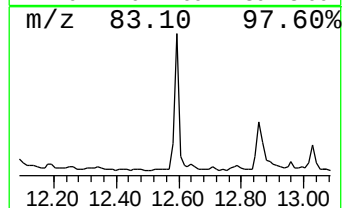
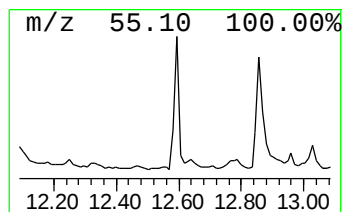
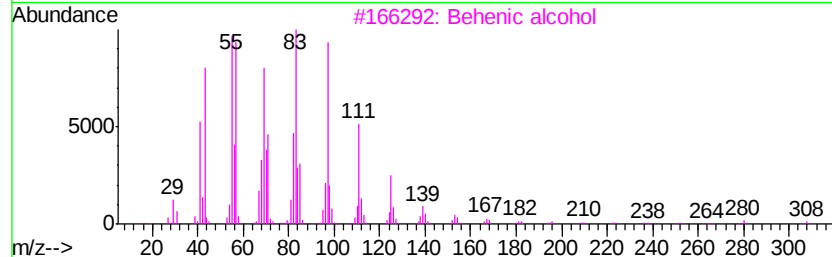
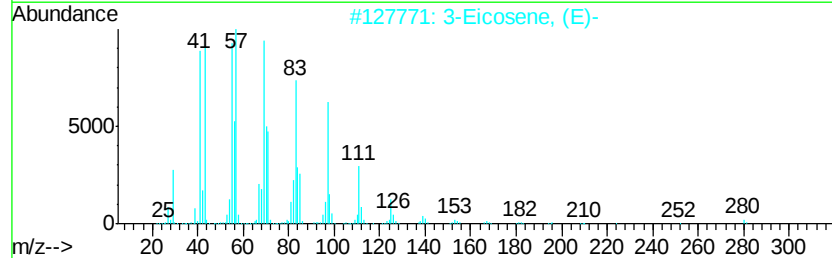
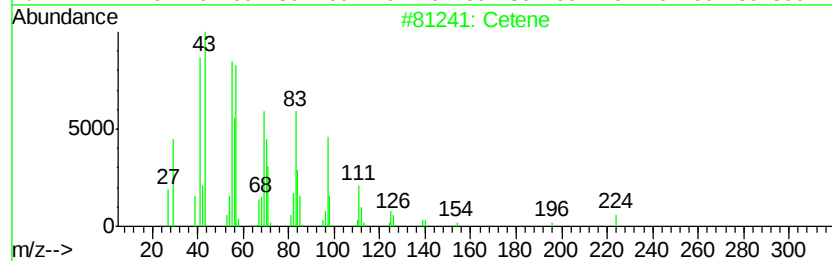
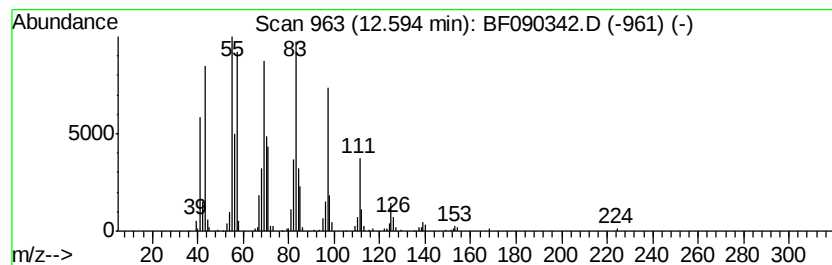
Instrument :
BNA_F
ClientSampleId :
SUP-B045-0-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Cetene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.59	2.39 ng	347119	Phenanthrene-d10	11.54
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Cetene	224 C16H32	000629-73-2	96
2	3-Eicosene, (E)-	280 C20H40	074685-33-9	95
3	Behenic alcohol	326 C22H46O	000661-19-8	94
4	n-Nonadecanol-1	284 C19H40O	001454-84-8	94
5	Chloroacetic acid, pentadecyl ester	304 C17H33ClO2	070301-47-2	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100416\
Data File : BF090342.D
Acq On : 4 Oct 2016 14:18
Operator : UM/SJ
Sample : H4998-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

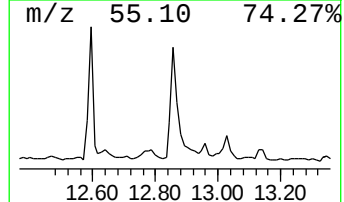
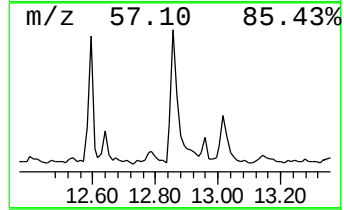
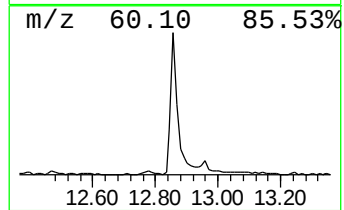
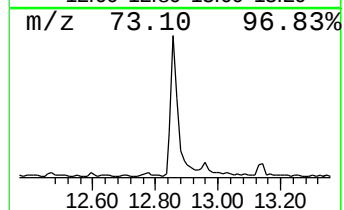
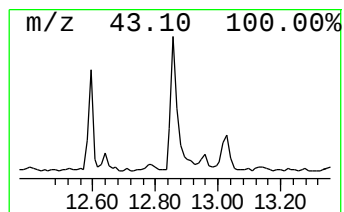
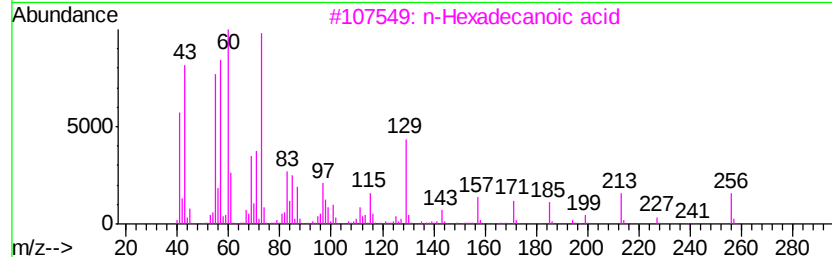
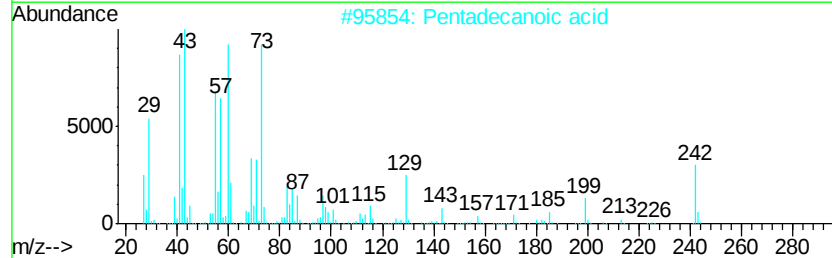
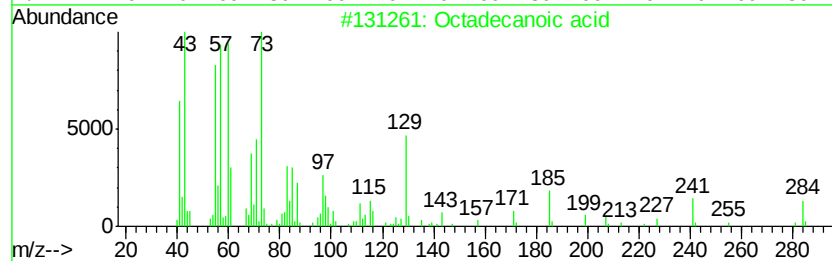
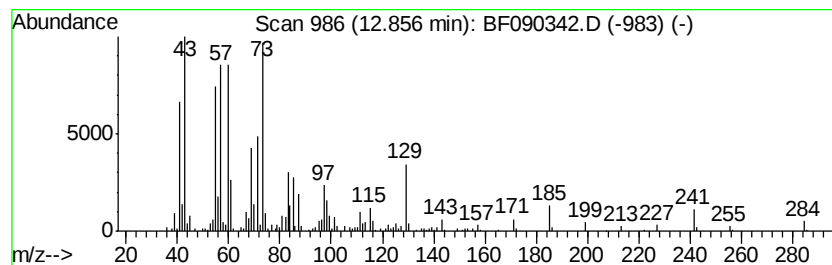
Instrument :
BNA_F
ClientSampleId :
SUP-B045-0-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.86	4.84 ng	701587	Phenanthrene-d10		11.54	
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	93
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4		Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	25
5		Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100416\
Data File : BF090342.D
Acq On : 4 Oct 2016 14:18
Operator : UM/SJ
Sample : H4998-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B045-0-3

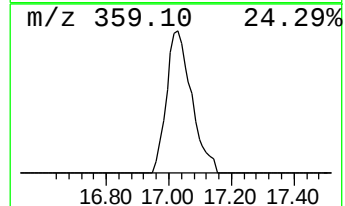
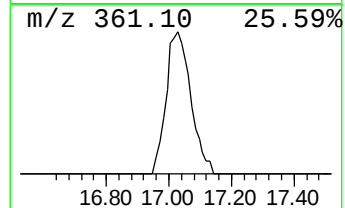
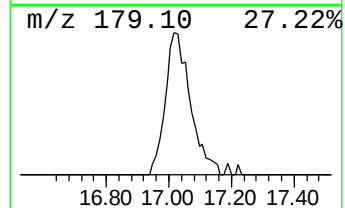
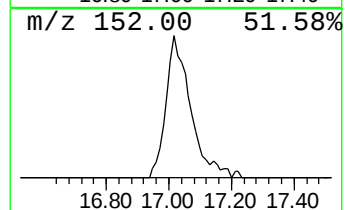
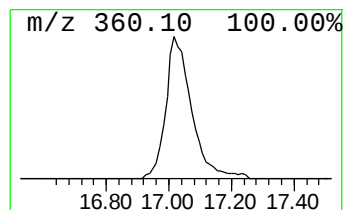
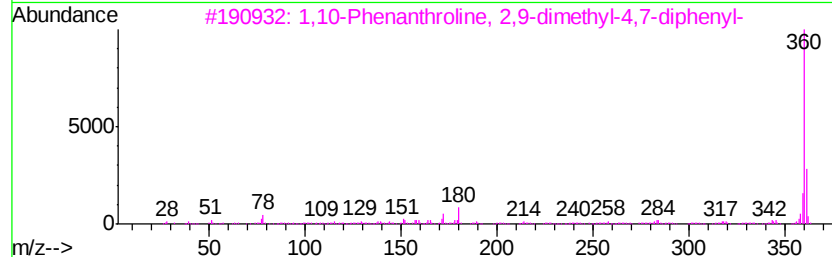
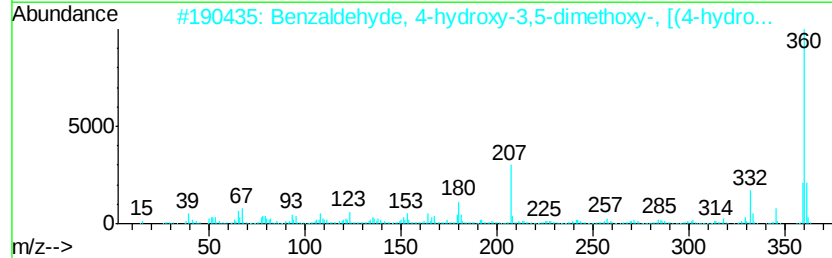
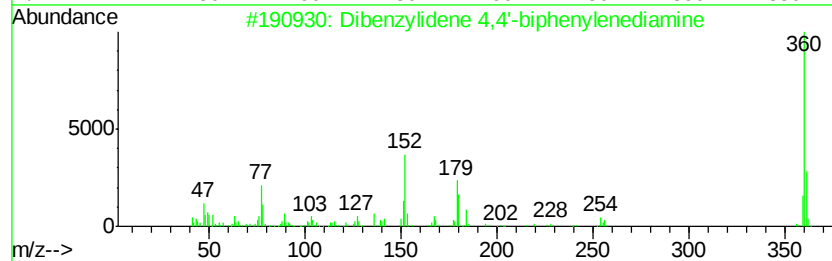
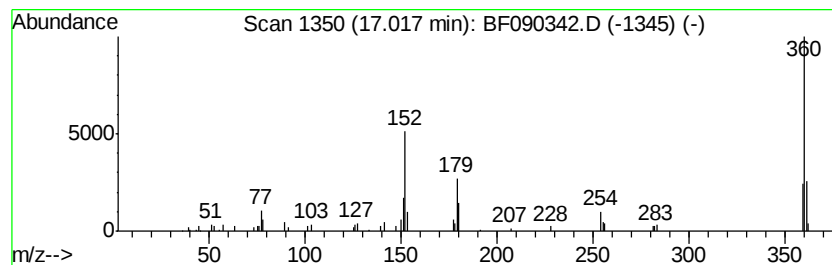
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Dibenzylidene 4,4'-biphenyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.02	3.23 ng	286995	Perylene-d12	15.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	87
2		Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	49
3		1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	43
4		1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13B06	1000150-23-7	43
5		Silane, dimethyl(4-bromophenoxy)...	358	C16H27BrO2Si	1000347-11-2	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100416\
Data File : BF090342.D
Acq On : 4 Oct 2016 14:18
Operator : UM/SJ
Sample : H4998-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B045-0-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	1.92	191.9	ng	18935900	1	7.00	1972980	20.0
2-Pentanone, 4-hy...	5.21	16.3	ng	1609940	1	7.00	1972980	20.0
unknown6.78	6.78	76.0	ng	7501540	1	7.00	1972980	20.0
2-Tetradecene, (E)-	11.77	3.9	ng	566590	4	11.54	2900700	20.0
n-Hexadecanoic acid	12.07	6.2	ng	900220	4	11.54	2900700	20.0
Cetene	12.59	2.4	ng	347119	4	11.54	2900700	20.0
Octadecanoic acid	12.86	4.8	ng	701587	4	11.54	2900700	20.0
Dibenzylidene 4,4...	17.02	3.2	ng	286995	6	15.70	1775410	20.0