

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121416\
 Data File : BF091602.D
 Acq On : 14 Dec 2016 23:31
 Operator : UM/SJ
 Sample : H6006-20
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-9-10-15

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-BF120916.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.967	249	252	260	rBV	1982169	2864100	36.99%	4.252%
2	5.356	284	286	287	rBV	106574	150239	1.94%	0.223%
3	5.401	287	290	292	rVB	6807930	6997737	90.37%	10.389%
4	6.441	378	381	383	rVB	6588281	7689931	99.31%	11.417%
5	6.567	389	392	394	rBV	7573629	7550607	97.51%	11.210%
6	6.796	409	412	414	rBV	2015755	1742581	22.50%	2.587%
7	6.956	423	426	428	rBV	5231771	5868440	75.78%	8.712%
8	7.356	458	461	464	rBV	3529536	4556769	58.85%	6.765%
9	8.076	522	524	527	rBV	2084052	2130916	27.52%	3.164%
10	9.162	616	619	621	rBV	8145379	7743557	100.00%	11.496%
11	9.550	651	653	656	rBV	873367	797439	10.30%	1.184%
12	9.836	675	678	680	rBV	2338391	2348293	30.33%	3.486%
13	10.248	712	714	715	rBV	126391	111882	1.44%	0.166%
14	10.270	715	716	718	rVB	110044	97140	1.25%	0.144%
15	10.625	744	747	749	rBV	3843118	4313334	55.70%	6.404%
16	10.750	756	758	762	rVB	113549	188282	2.43%	0.280%
17	11.196	795	797	798	rBV	156082	154076	1.99%	0.229%
18	11.310	805	807	810	rVB	1818609	1894409	24.46%	2.812%
19	11.551	825	828	832	rBV2	73796	103323	1.33%	0.153%
20	11.619	832	834	837	rVB	196449	170832	2.21%	0.254%
21	11.848	853	854	856	rBV2	122590	152638	1.97%	0.227%
22	12.031	868	870	871	rVB	72305	84079	1.09%	0.125%
23	12.751	929	933	935	rBV2	42721	84068	1.09%	0.125%
24	12.899	943	946	949	rBV	4938212	4960680	64.06%	7.365%
25	13.391	986	989	991	rBV	235249	327530	4.23%	0.486%
26	13.802	1023	1025	1029	rVB2	250040	312737	4.04%	0.464%
27	13.951	1035	1038	1040	rBV	1389532	1676014	21.64%	2.488%
28	14.431	1078	1080	1082	rBV	84105	85436	1.10%	0.127%
29	15.357	1158	1161	1164	rBV	1043674	1435562	18.54%	2.131%
30	15.402	1164	1165	1168	rVB	89103	103098	1.33%	0.153%
31	15.814	1199	1201	1203	rBV	121285	180144	2.33%	0.267%
32	16.282	1240	1242	1247	rVB	139467	270217	3.49%	0.401%
33	16.831	1288	1290	1294	rVB	104025	210960	2.72%	0.313%

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Instrument :
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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-BF120916.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

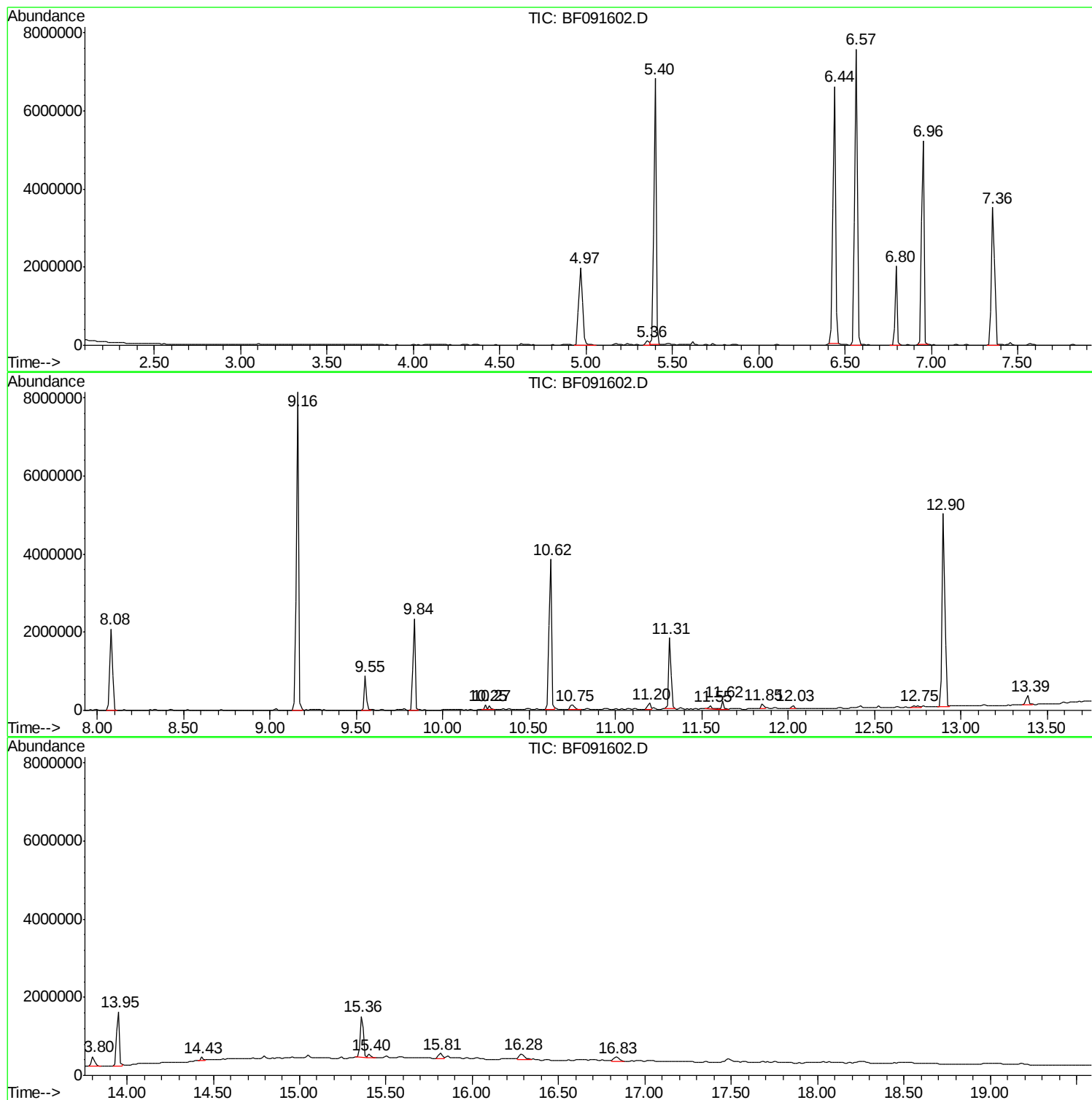
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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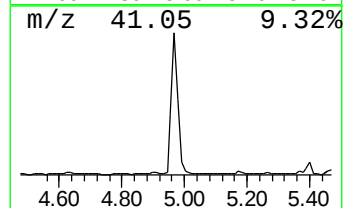
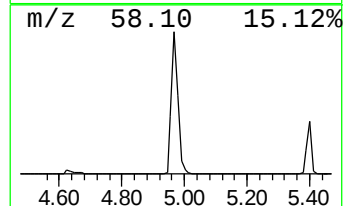
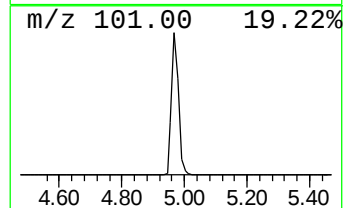
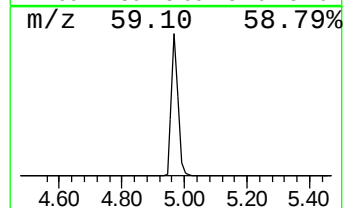
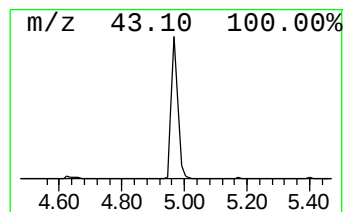
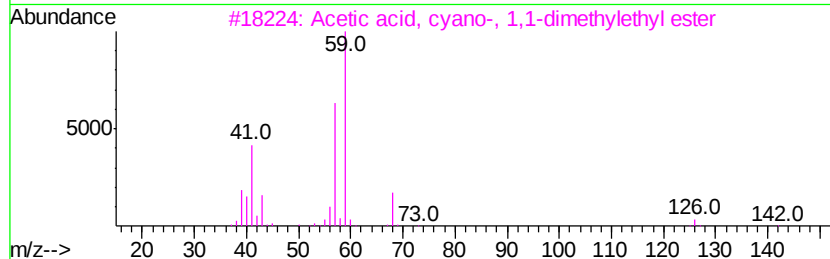
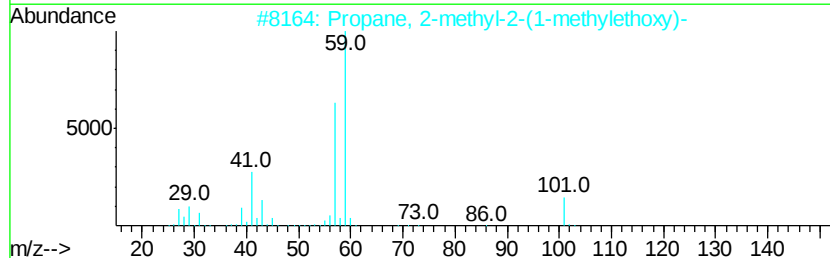
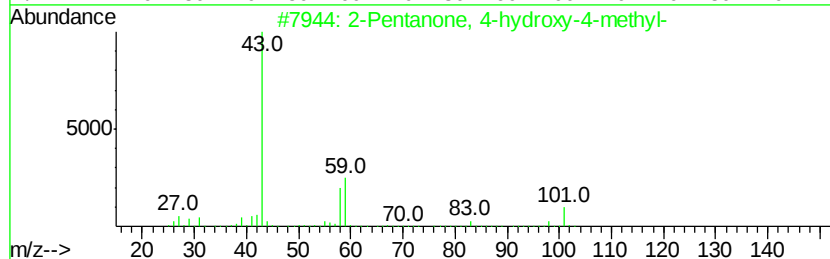
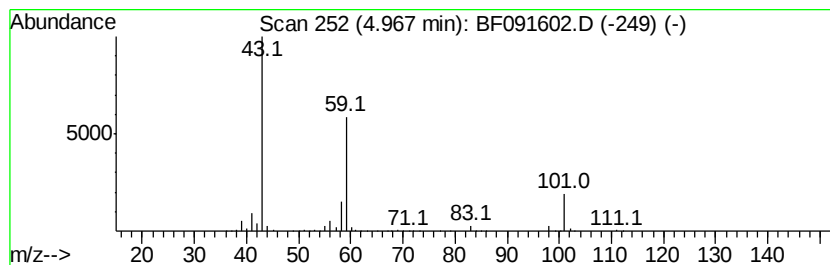
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	32.87 ng	2864100	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	28
3		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	25
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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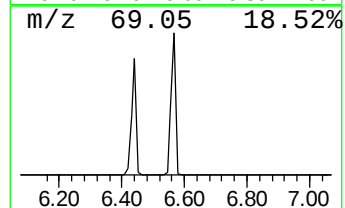
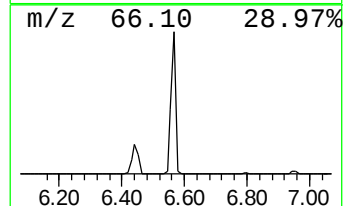
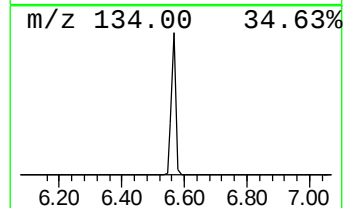
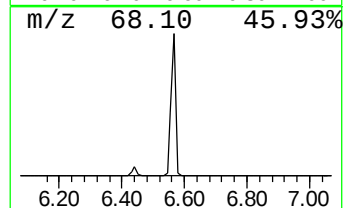
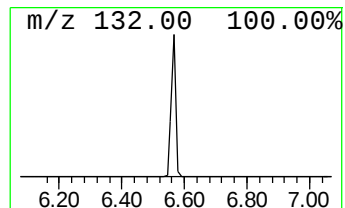
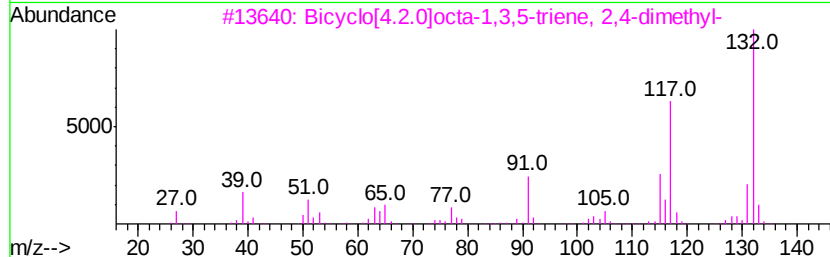
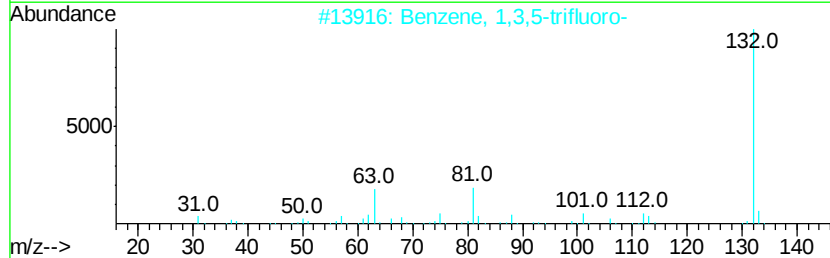
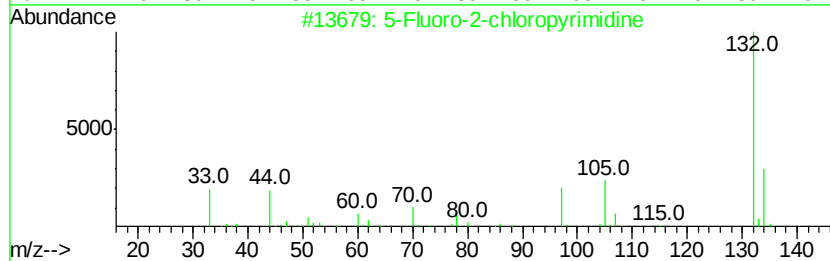
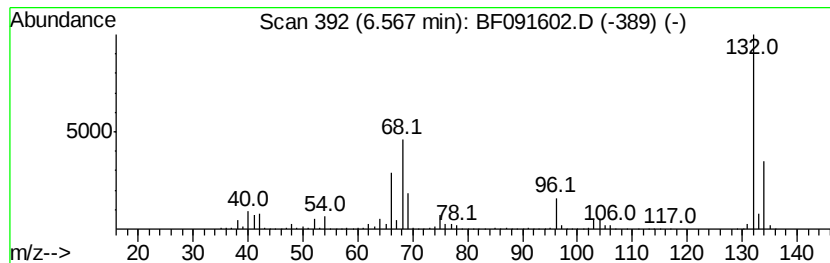
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	86.66 ng	7550610	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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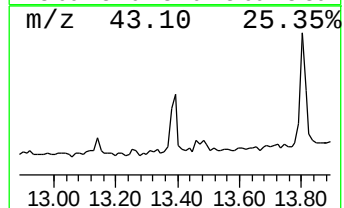
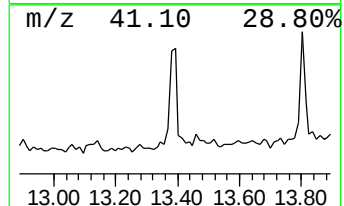
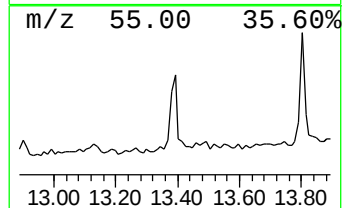
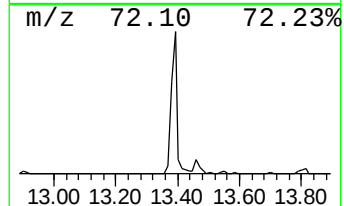
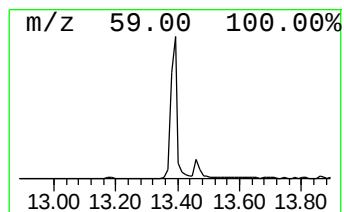
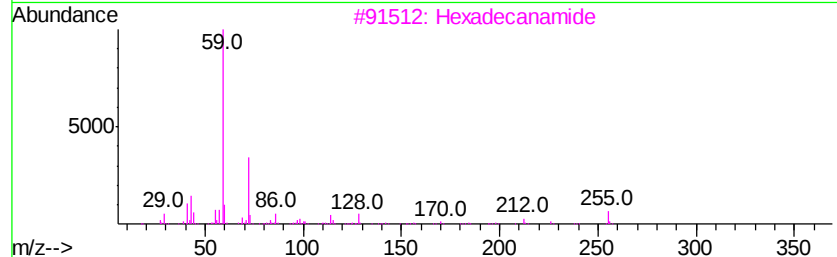
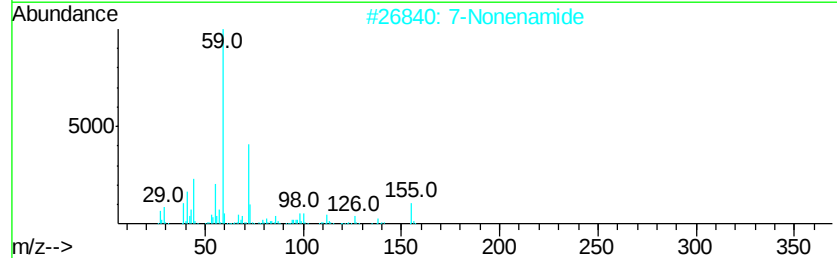
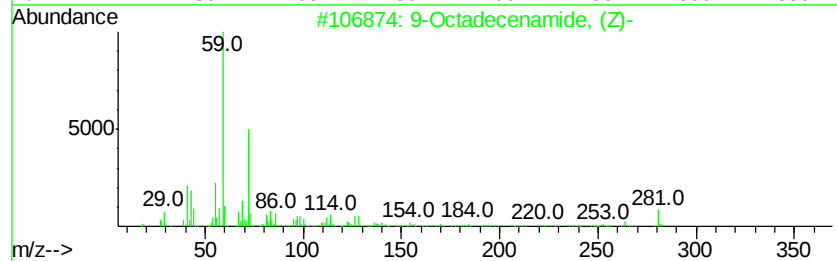
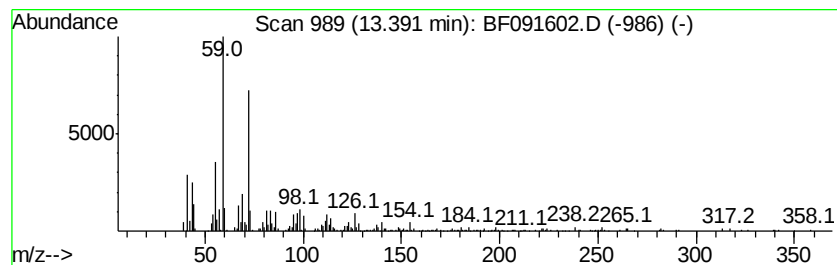
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.39	3.91 ng	327530	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2		7-Nonenamide	155	C9H17NO	090949-53-4	72
3		Hexadecanamide	255	C16H33NO	000629-54-9	64
4		Decanamide-	171	C10H21NO	002319-29-1	59
5		Silane, hexyl-	116	C6H16Si	001072-14-6	50



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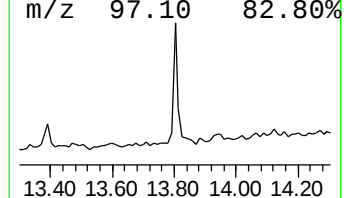
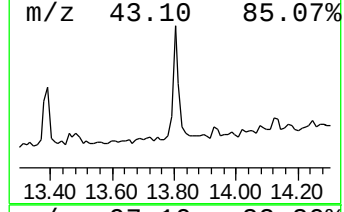
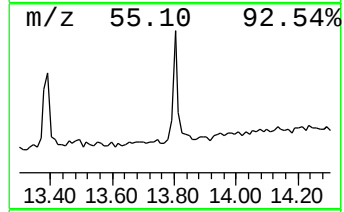
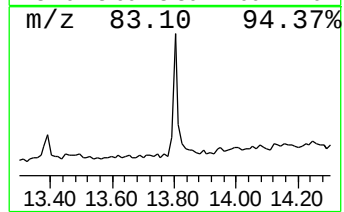
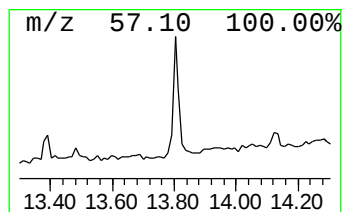
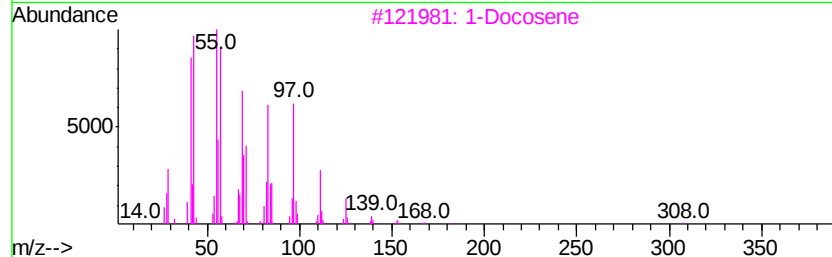
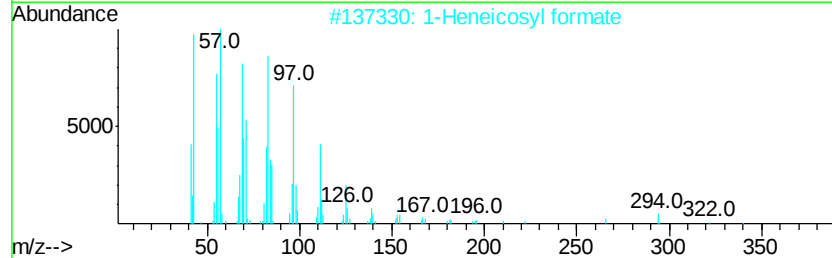
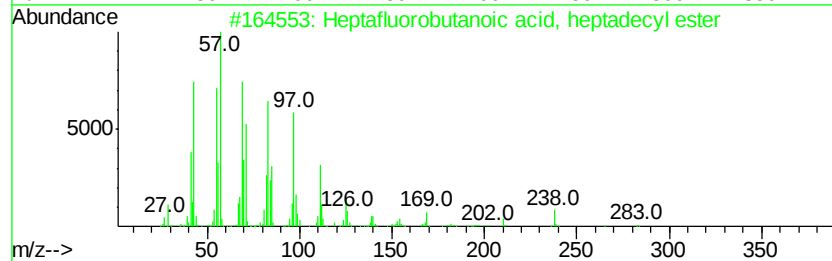
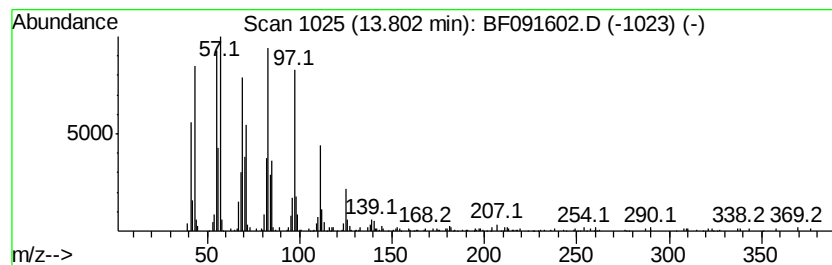
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptafluorobutanoic acid, h... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.80	3.73 ng	312737	Chrysene-d12	13.95		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutanoic acid, heptadecanoic acid	452	C21H35F7O2	1000282-97-3	94
2		1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3		1-Docosene	308	C22H44	001599-67-3	91
4		Trifluoroacetic acid, n-octadecanoic acid	366	C20H37F3O2	079392-43-1	91
5		2-Chloropropionic acid, hexadecanoic acid	332	C19H37ClO2	086711-81-1	91



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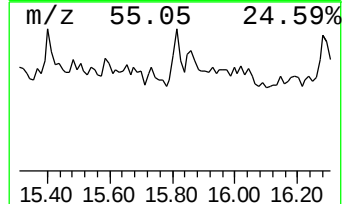
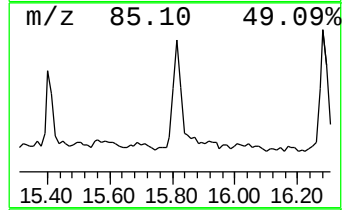
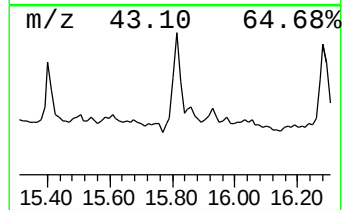
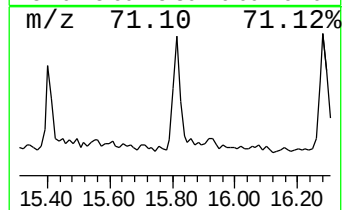
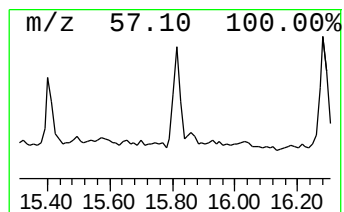
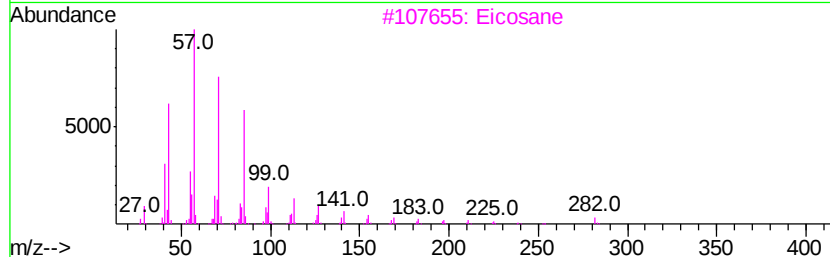
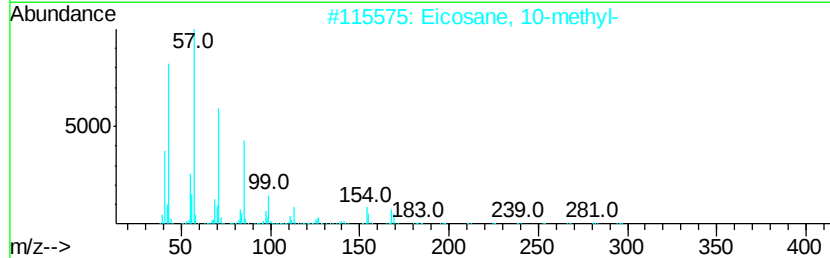
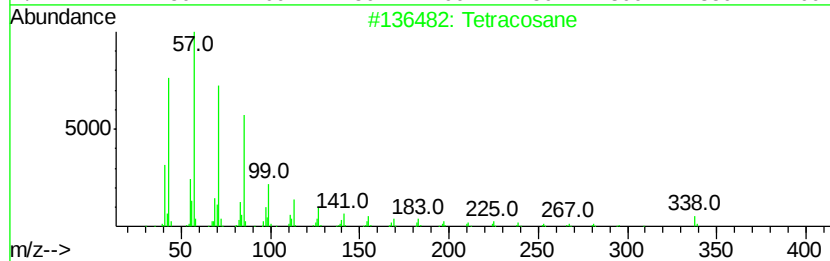
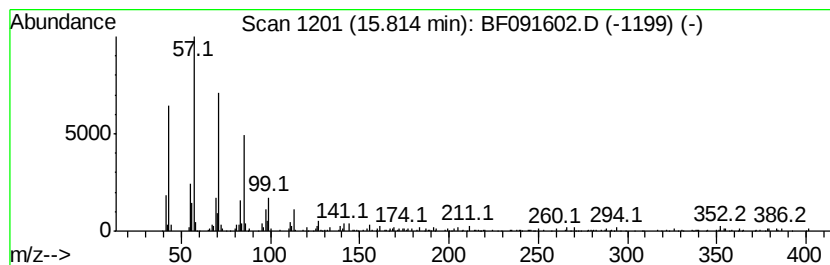
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Peak Number 6 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.81	2.51 ng	180144	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	95
2		Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
3		Eicosane	282	C20H42	000112-95-8	93
4		2-Bromo dodecane	248	C12H25Br	013187-99-0	93
5		Octacosane	394	C28H58	000630-02-4	87



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Sample : H6006-20
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-9-10-15

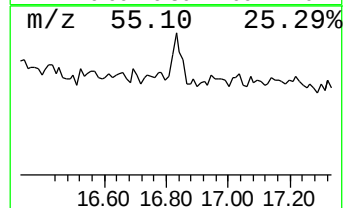
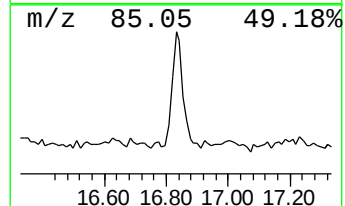
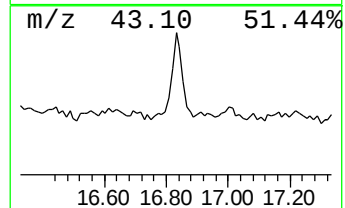
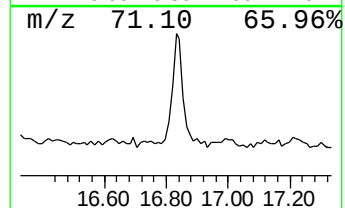
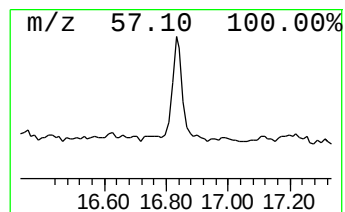
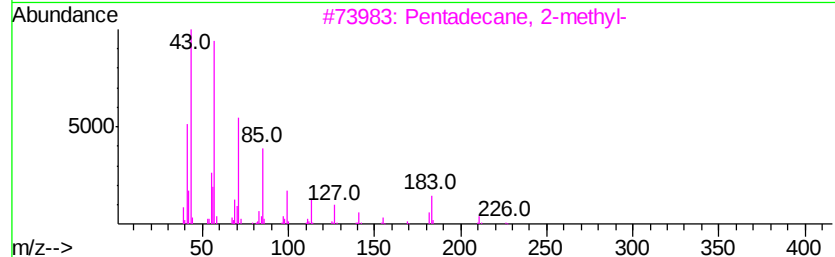
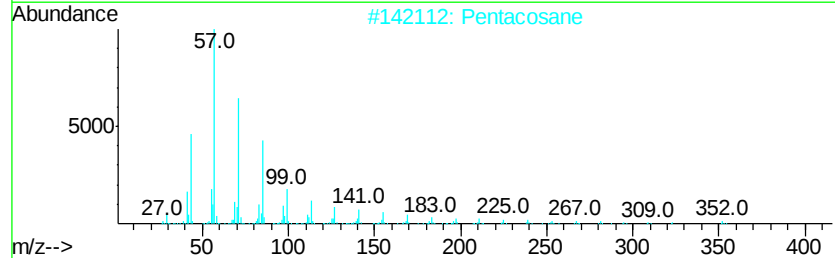
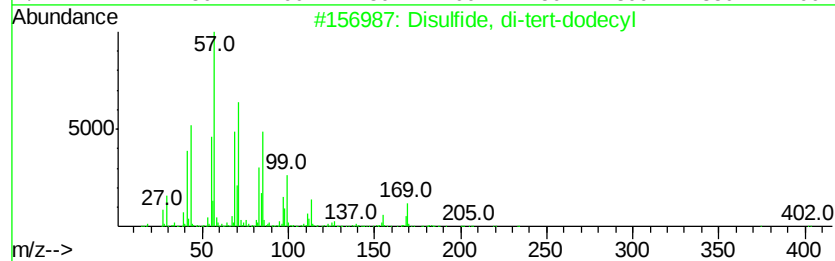
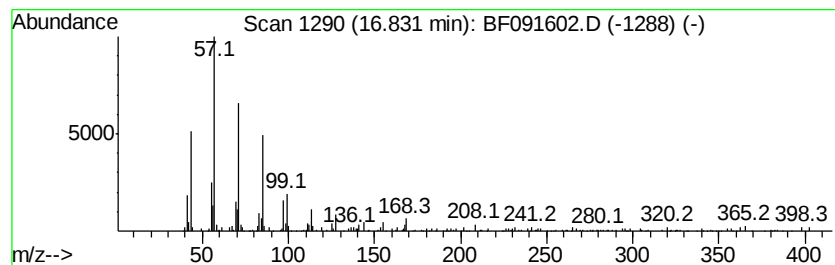
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Disulfide, di-tert-dodecyl Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.83	2.94 ng	210960	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	90
2		Pentacosane	352	C25H52	000629-99-2	83
3		Pentadecane, 2-methyl-	226	C16H34	001560-93-6	83
4		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	80
5		Docosane	310	C22H46	000629-97-0	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121416\
Data File : BF091602.D
Acq On : 14 Dec 2016 23:31
Operator : UM/SJ
Sample : H6006-20
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-9-10-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.97	32.9	ng	2864100	1	6.80	1742580	20.0
unknown6.57	6.57	86.7	ng	7550610	1	6.80	1742580	20.0
9-Octadecenamide, ...	13.39	3.9	ng	327530	5	13.95	1676010	20.0
Heptafluorobutano...	13.80	3.7	ng	312737	5	13.95	1676010	20.0
Tetracosane	15.81	2.5	ng	180144	6	15.36	1435560	20.0
Disulfide, di-ter...	16.83	2.9	ng	210960	6	15.36	1435560	20.0