

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061416\
 Data File : BF088032.D
 Acq On : 15 Jun 2016 7:43
 Operator : UM/SJ
 Sample : H3473-11
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 STA-1100-(0-4)

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-BF060716.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	1.724	10	12	13	rBV	267439	374054	5.87%	1.206%
2	1.850	21	23	26	rBV	660404	1275598	20.02%	4.113%
3	2.547	82	84	88	rVB	76994	98780	1.55%	0.319%
4	3.290	145	149	153	rBV	143657	266004	4.17%	0.858%
5	4.330	234	240	243	rBV	2589176	6372385	100.00%	20.547%
6	4.970	293	296	305	rVB	173915	322898	5.07%	1.041%
7	5.393	330	333	335	rBV	1841124	2300761	36.11%	7.419%
8	6.422	421	423	426	rBV	1637108	1945575	30.53%	6.273%
9	6.559	432	435	437	rBV	1708534	2409848	37.82%	7.770%
10	6.787	452	455	457	rBV	426804	583136	9.15%	1.880%
11	6.936	466	468	471	rVB	1820613	1849904	29.03%	5.965%
12	7.302	497	500	501	rVB	52495	65078	1.02%	0.210%
13	7.348	501	504	507	rBV	1394565	1412092	22.16%	4.553%
14	8.068	565	567	571	rBV2	975921	1452038	22.79%	4.682%
15	9.153	659	662	664	rBV	2602112	2947868	46.26%	9.505%
16	9.828	718	721	722	rBV	548677	762485	11.97%	2.459%
17	10.605	787	789	792	rBV2	1009446	1355437	21.27%	4.370%
18	11.302	848	850	852	rBV	824185	699093	10.97%	2.254%
19	12.022	910	913	915	rBV	117228	171362	2.69%	0.553%
20	12.719	971	974	976	rBV	501533	409951	6.43%	1.322%
21	12.799	976	981	983	rVB2	45537	77637	1.22%	0.250%
22	12.891	986	989	991	rBV	2239231	2128098	33.40%	6.862%
23	13.417	1033	1035	1038	rBV2	201260	261051	4.10%	0.842%
24	13.474	1038	1040	1043	rVB	33046	72572	1.14%	0.234%
25	13.931	1078	1080	1083	rBV	671384	658598	10.34%	2.124%
26	14.114	1093	1096	1098	rBV	73966	68150	1.07%	0.220%
27	14.708	1146	1148	1151	rBV	68542	70677	1.11%	0.228%
28	15.337	1201	1203	1205	rBV	314017	433094	6.80%	1.396%
29	15.383	1205	1207	1211	rVB	56151	71458	1.12%	0.230%
30	16.023	1258	1263	1266	rBV	55931	97815	1.53%	0.315%

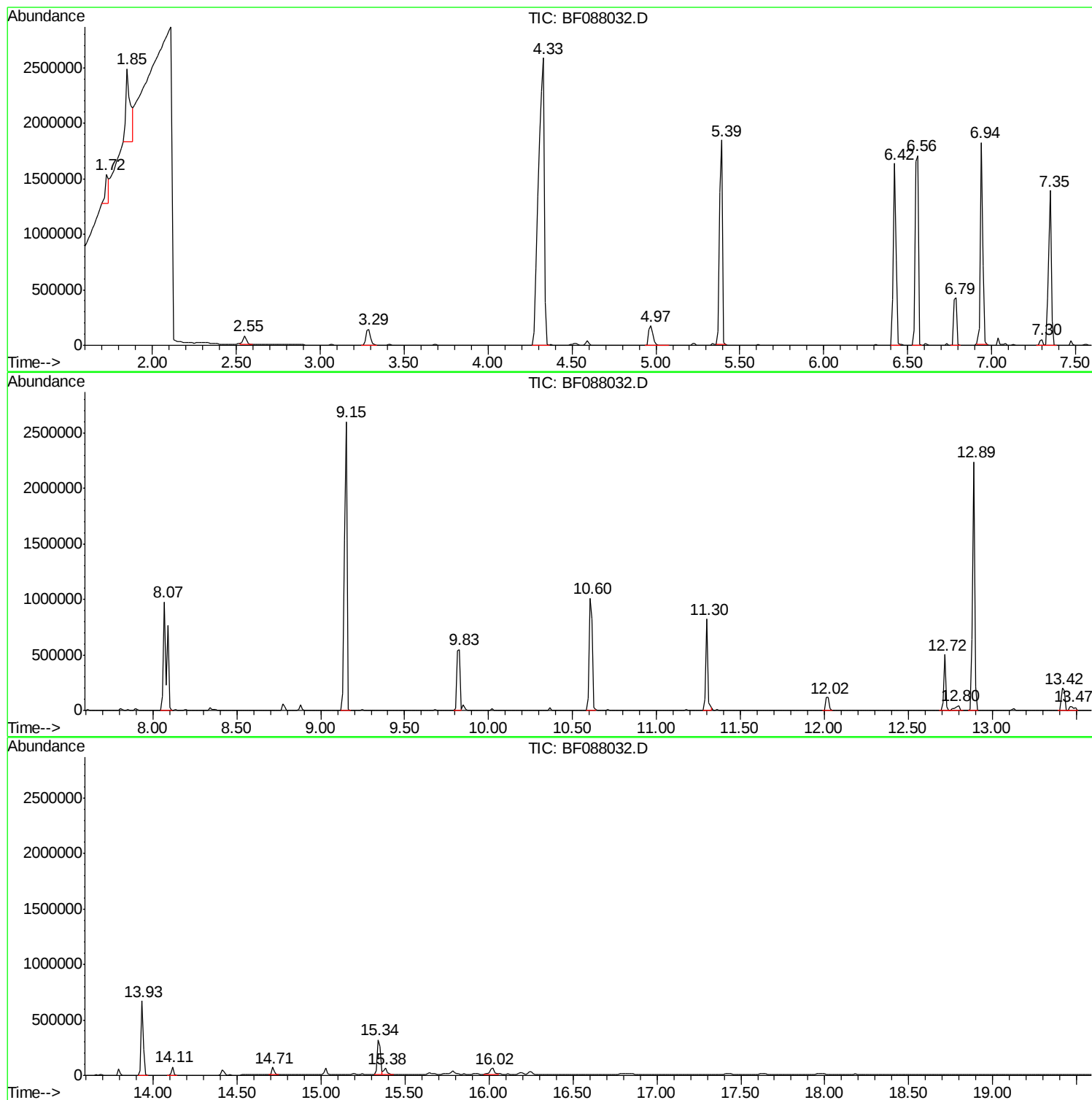
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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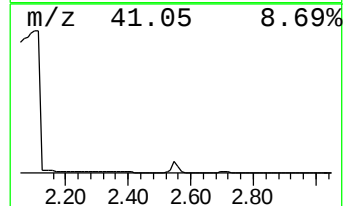
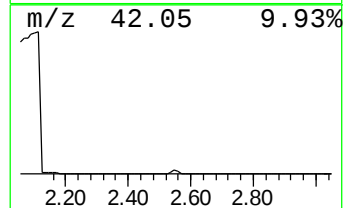
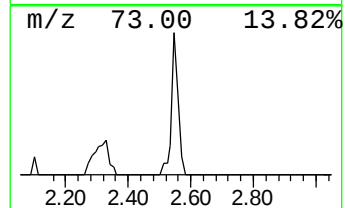
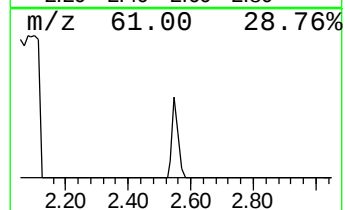
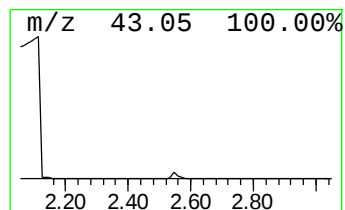
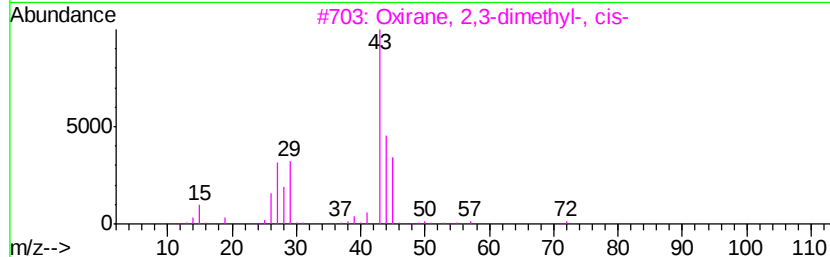
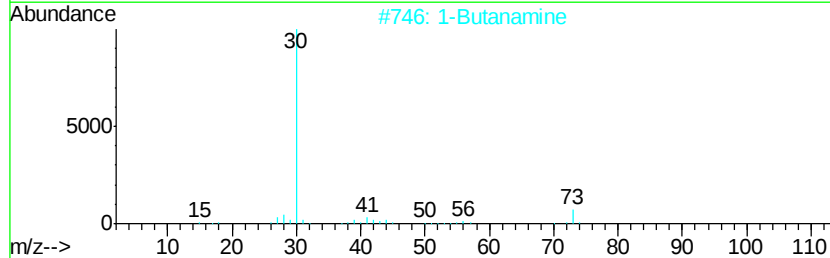
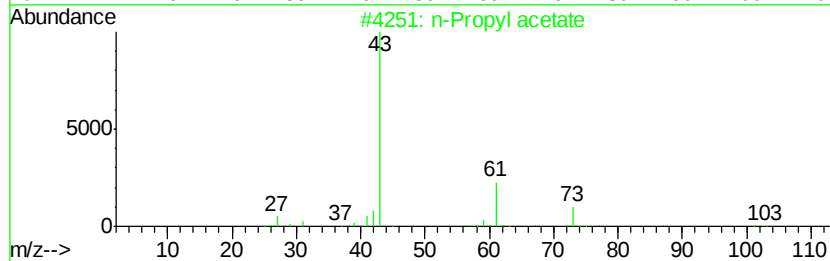
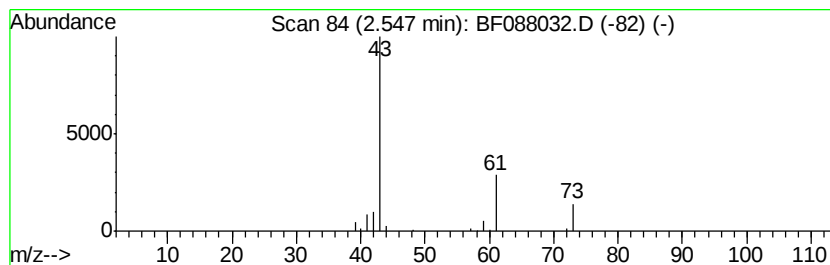
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Propyl acetate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.55	3.39 ng	98780	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2		1-Butanamine	73	C4H11N	000109-73-9	7
3		Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	7
4		Isobutylamine	73	C4H11N	000078-81-9	5
5		Acetic acid, pentyl ester	130	C7H14O2	000628-63-7	4



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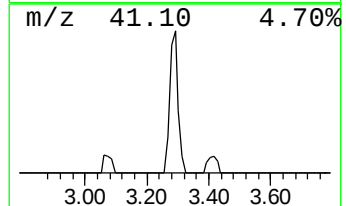
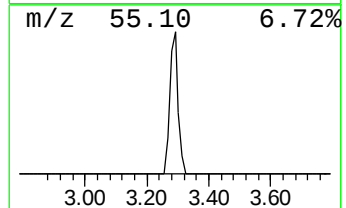
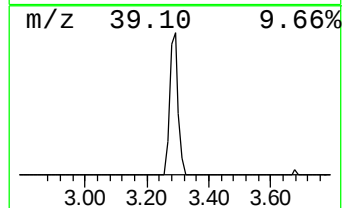
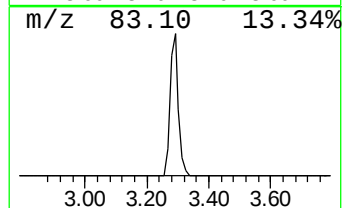
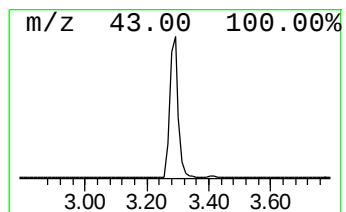
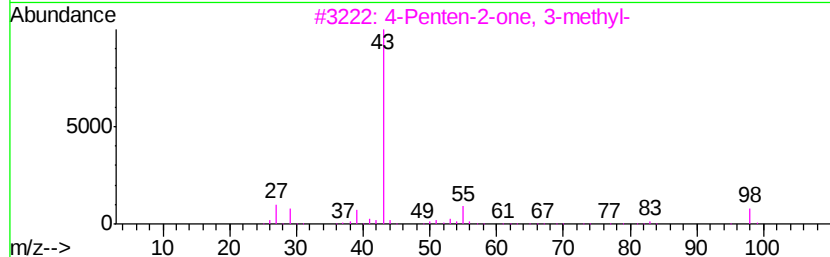
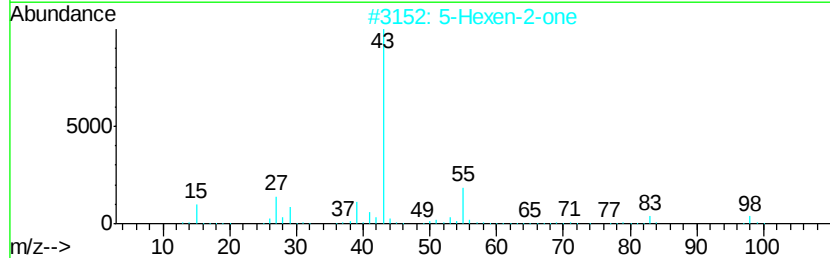
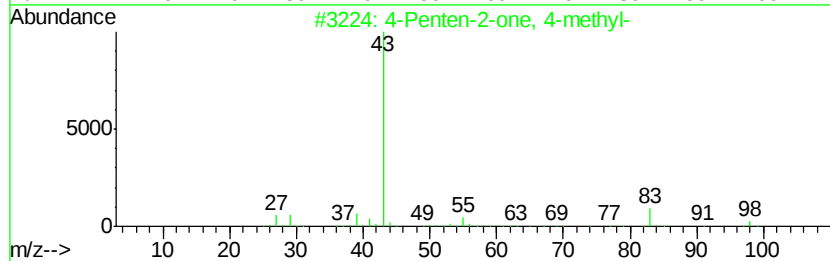
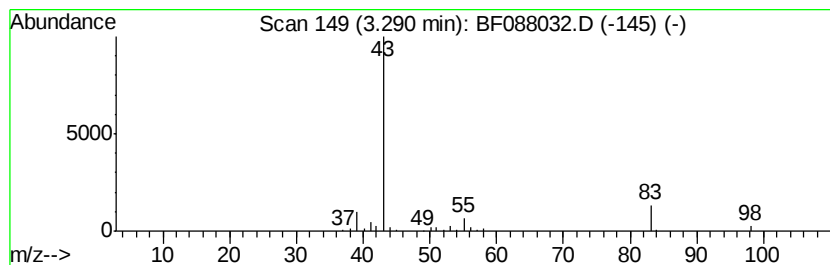
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Peak Number 4 4-Penten-2-one, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.29	9.12 ng	266004	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	86
2		5-Hexen-2-one	98	C6H10O	000109-49-9	50
3		4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	38
4		2-Pentanone, 3-methyl-	98	C6H10O	004359-77-7	23
5		4-Hexen-2-one	98	C6H10O	025659-22-7	9



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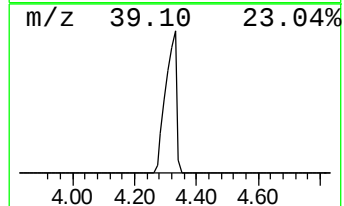
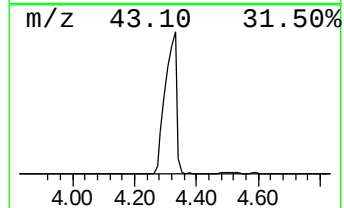
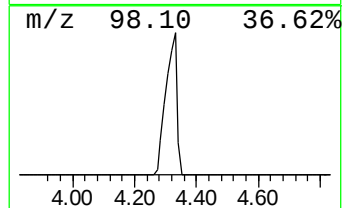
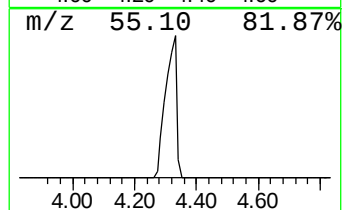
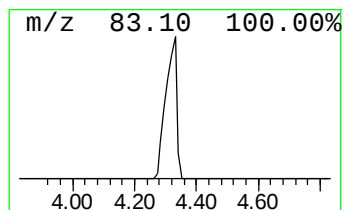
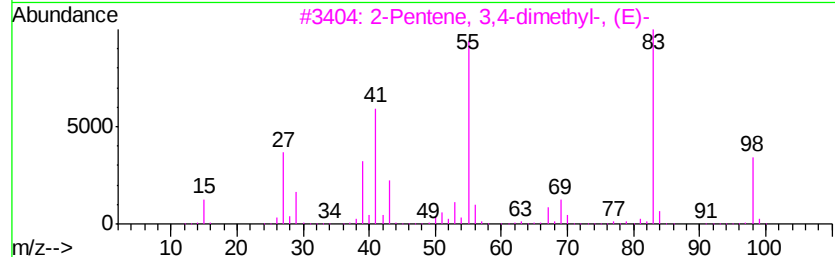
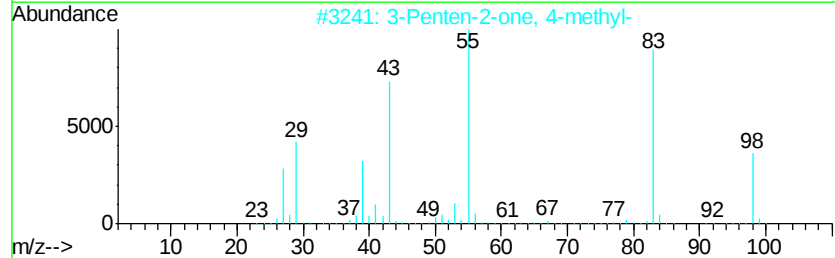
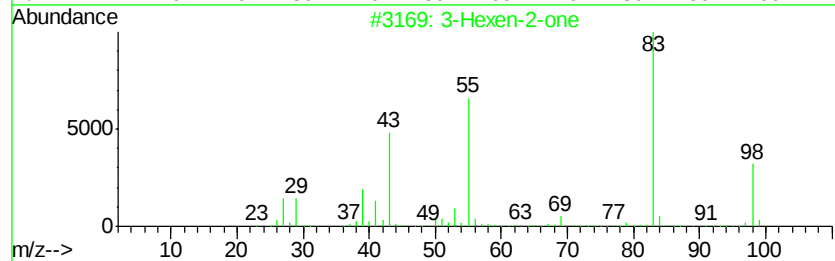
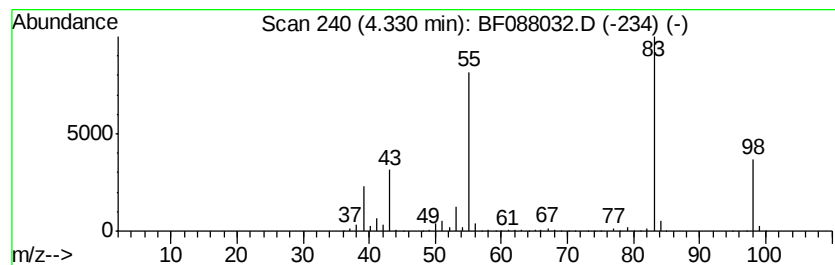
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Peak Number 5 3-Hexen-2-one Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.33	218.56 ng	6372390	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78



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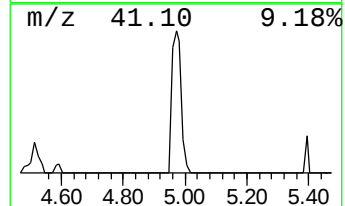
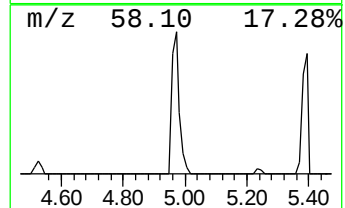
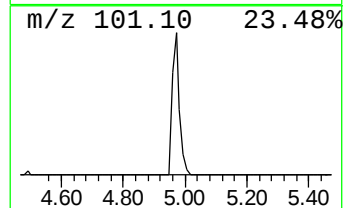
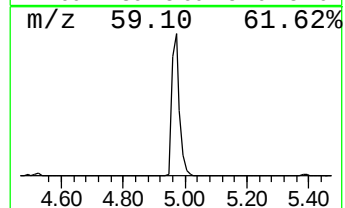
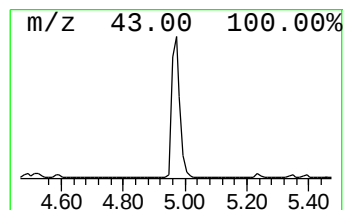
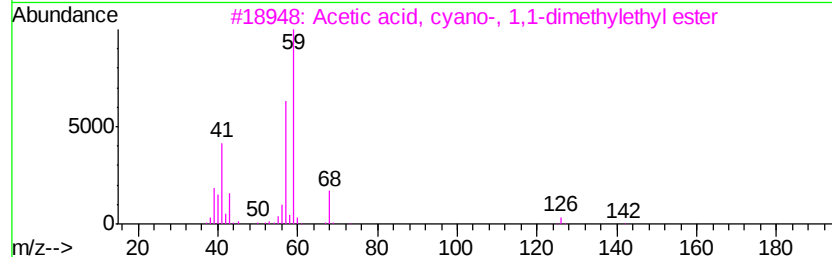
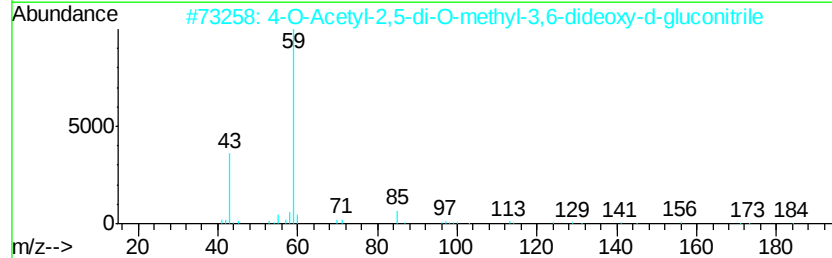
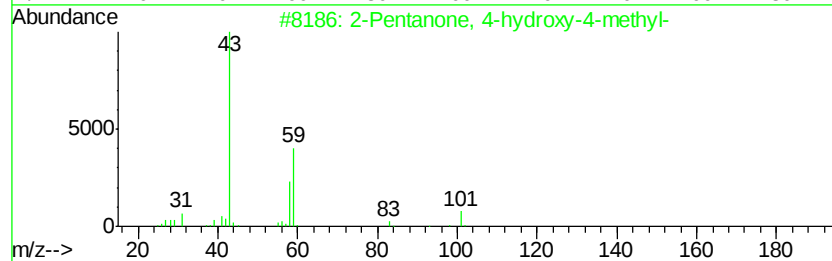
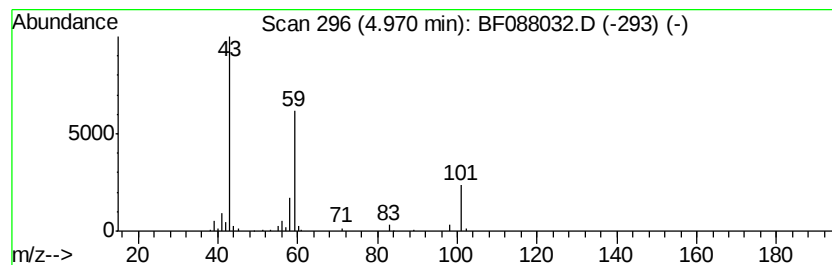
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	11.07 ng	322898	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		4-O-Acetyl-2,5-di-O-methyl-3,6-d...	215	C10H17NO4	1000101-80-3	17
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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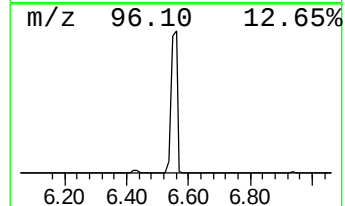
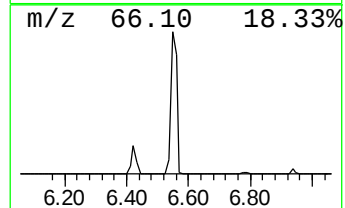
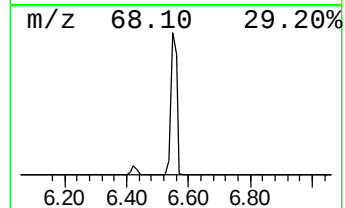
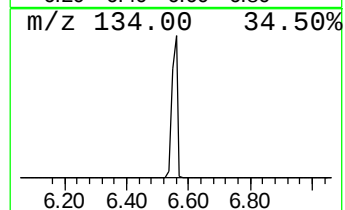
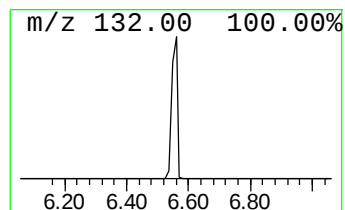
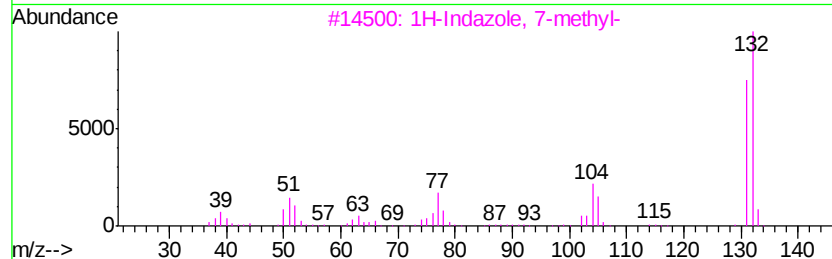
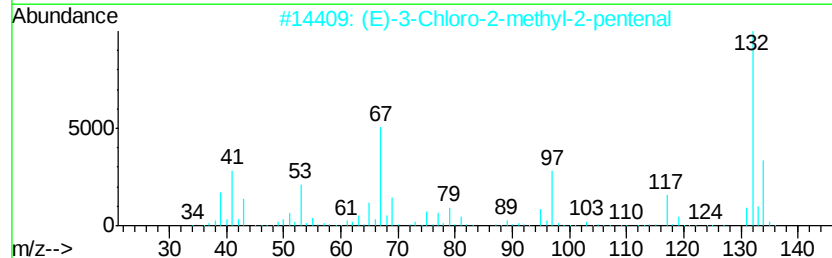
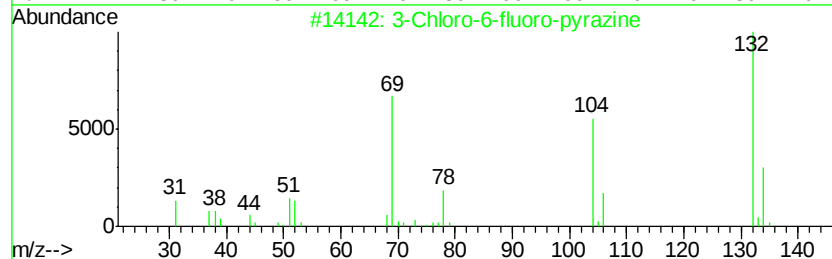
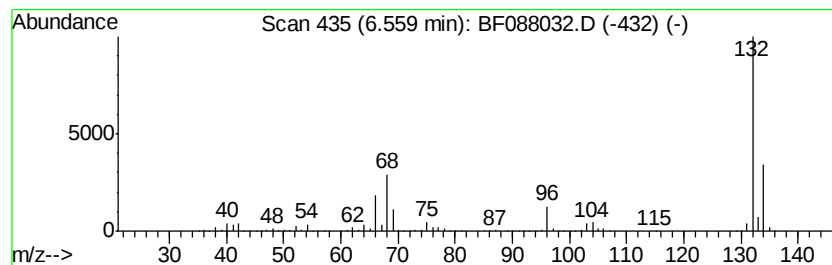
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Peak Number 7 unknown6.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	82.65 ng	2409850	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	40
2	(E)-3-Chloro-2-methyl-2-pentenal			132	C6H9ClO	031357-76-3	33
3	1H-Indazole, 7-methyl-			132	C8H8N2	1000316-00-7	25
4	4-Chloro-2-fluoro-pyrimidine			132	C4H2ClFN2	051422-00-5	9
5	4-Chloro-6-fluoro-pyrimidine			132	C4H2ClFN2	051422-01-6	9



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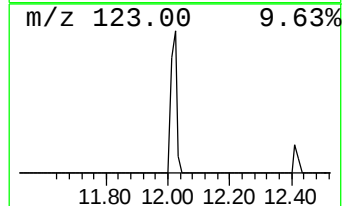
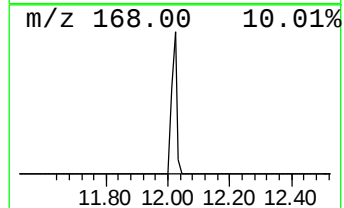
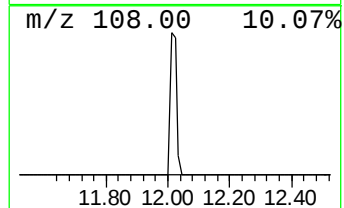
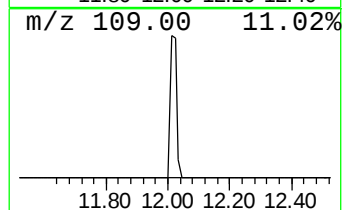
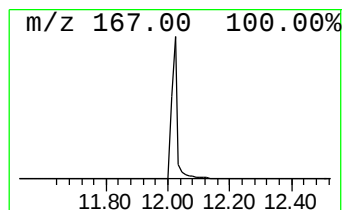
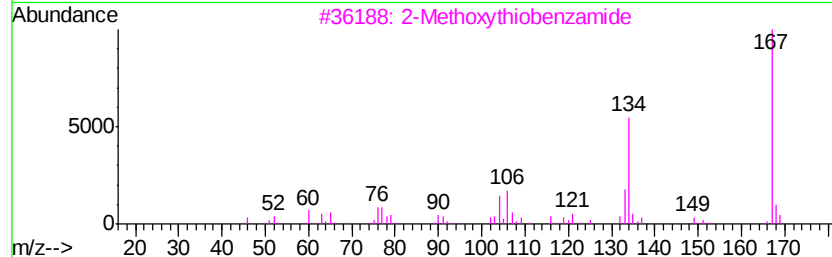
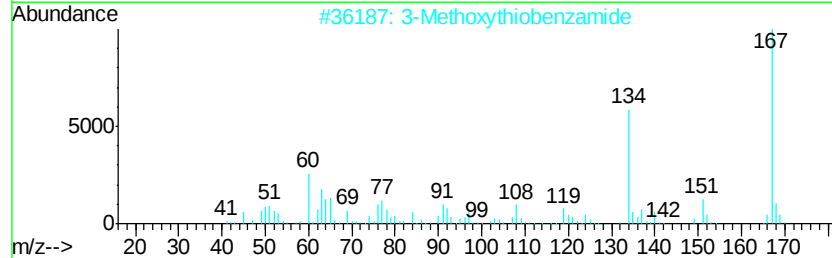
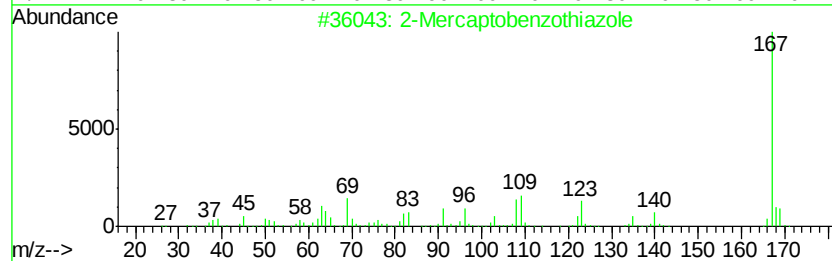
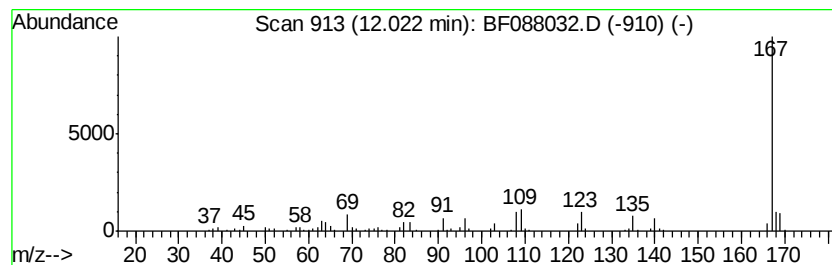
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-Mercaptobenzothiazole Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	4.90 ng	171362	Phenanthrene-d10	11.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	95
2		3-Methoxythiobenzamide	167	C8H9NOS	064559-06-4	59
3		2-Methoxythiobenzamide	167	C8H9NOS	042590-97-6	53
4		2',4'-Dihydroxyacetophenone oxime	167	C8H9NO3	1000212-89-5	47
5		Thioguanine	167	C5H5N5S	000154-42-7	42



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061416\
Data File : BF088032.D
Acq On : 15 Jun 2016 7:43
Operator : UM/SJ
Sample : H3473-11
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STA-1100-(0-4)

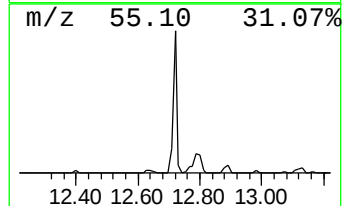
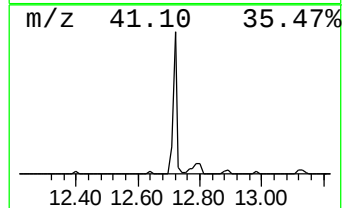
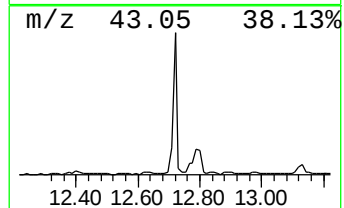
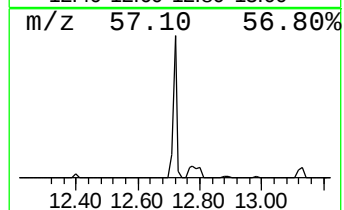
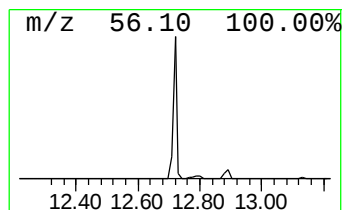
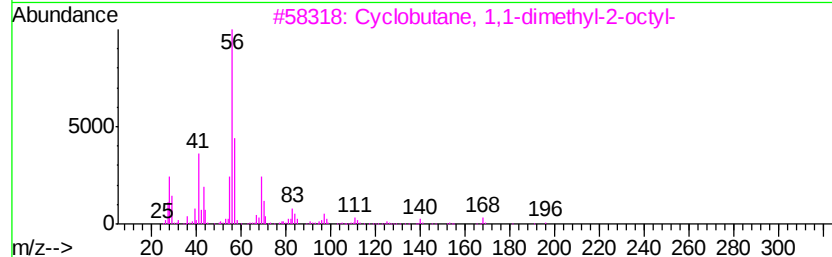
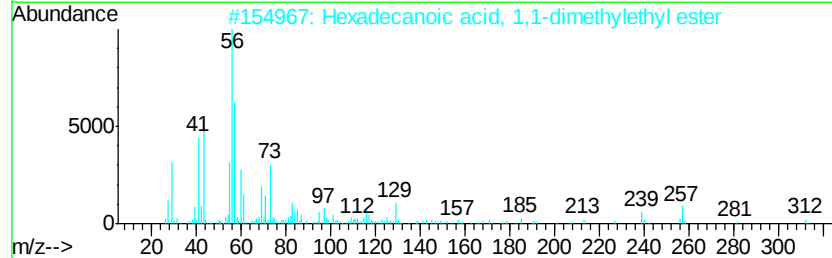
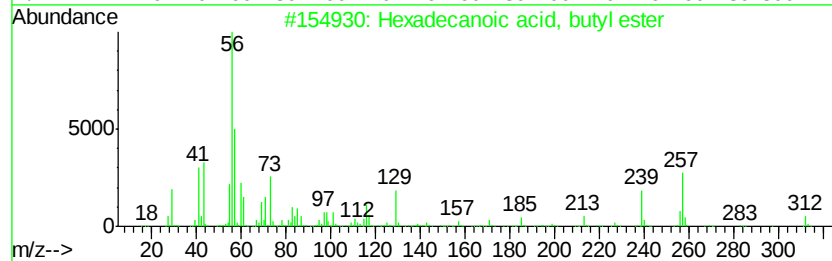
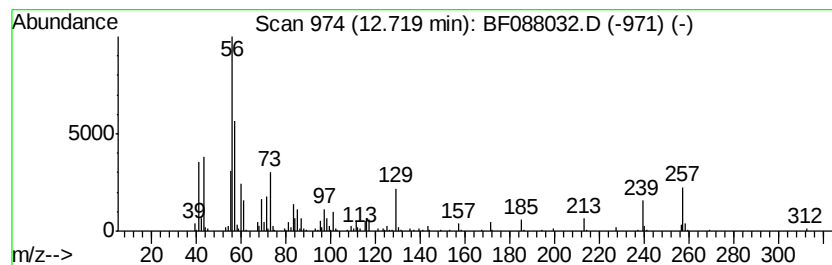
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	12.45 ng	409951	Chrysene-d12	13.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	74
3		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
4		Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	35
5		1-Hexene, 4-methyl-	98	C7H14	003769-23-1	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061416\
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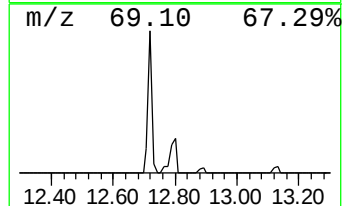
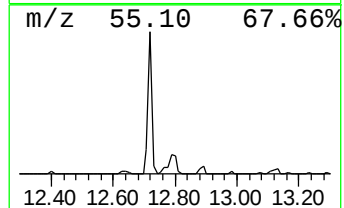
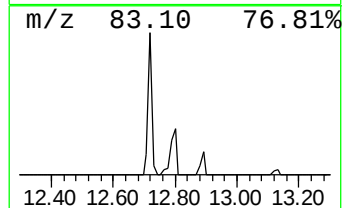
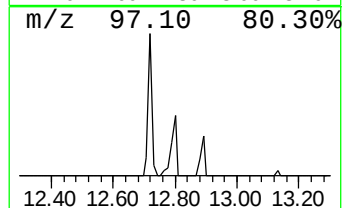
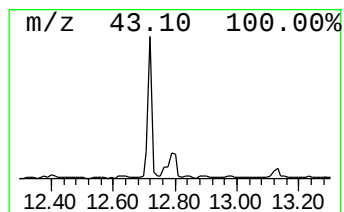
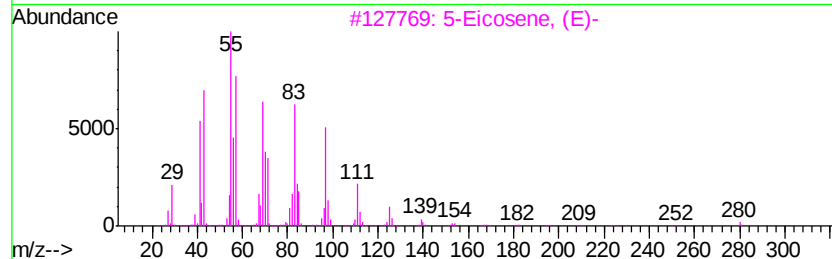
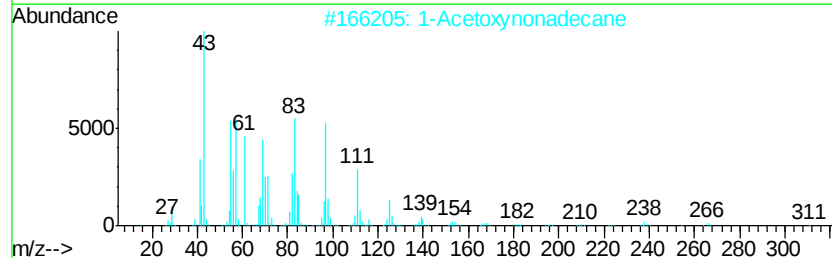
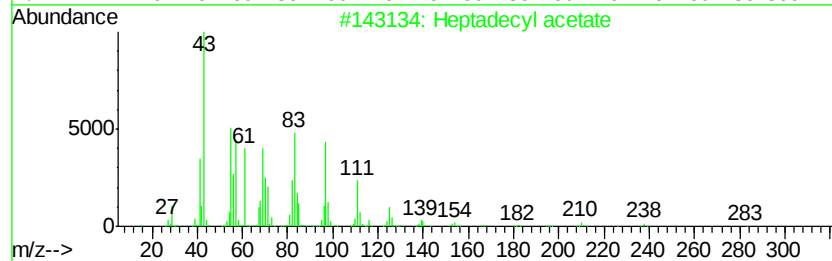
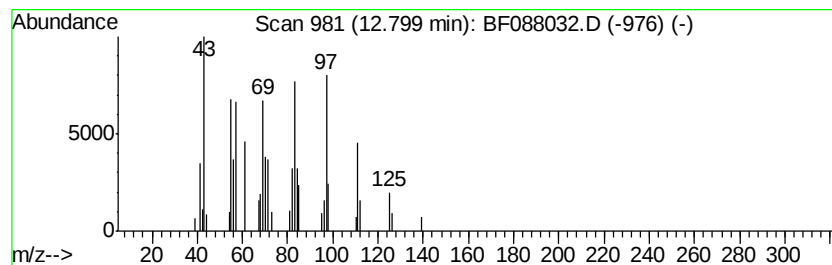
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptadecyl acetate Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	2.36 ng	77637	Chrysene-d12	13.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl acetate	298	C19H38O2	000822-20-8	91
2		1-Acetoxynonadecane	326	C21H42O2	001577-43-1	91
3		5-Eicosene, (E)-	280	C20H40	074685-30-6	90
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	87
5		1-Docosene	308	C22H44	001599-67-3	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061416\
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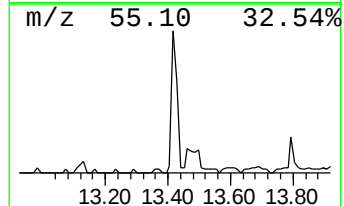
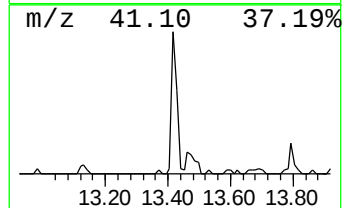
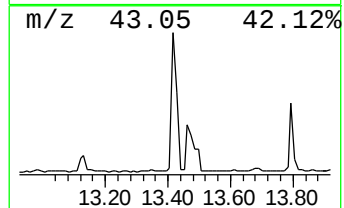
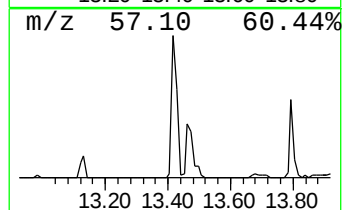
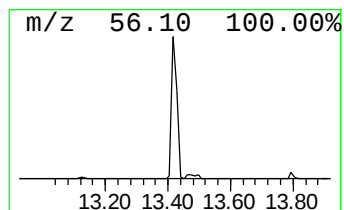
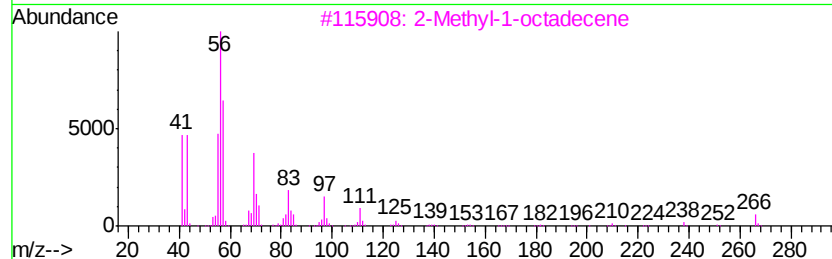
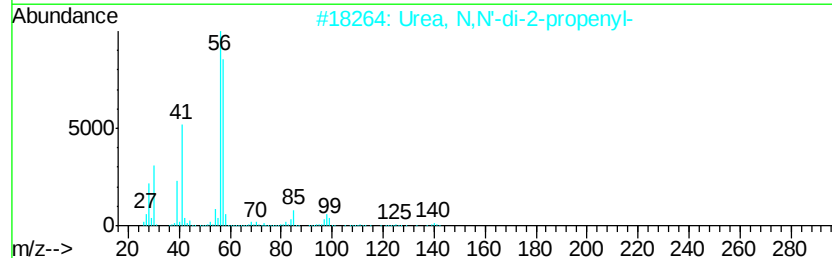
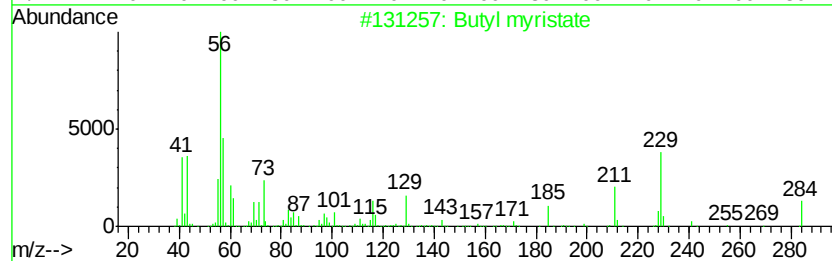
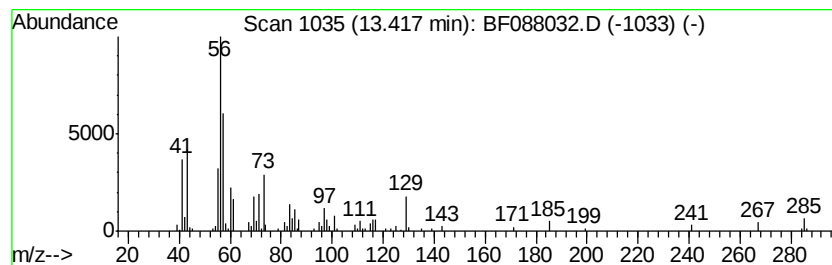
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Butyl myristate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.42	7.93 ng	261051	Chrysene-d12		13.93
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	80
2	Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	38
3	2-Methyl-1-octadecene	266	C19H38	061868-20-0	38
4	Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	35
5	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061416\
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Acq On : 15 Jun 2016 7:43
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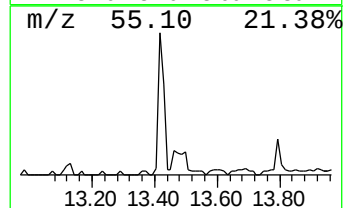
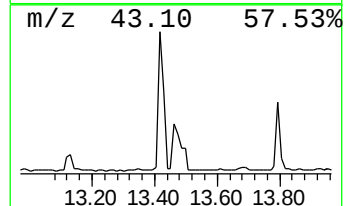
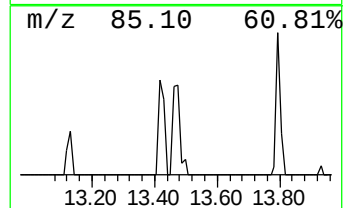
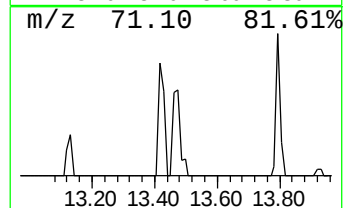
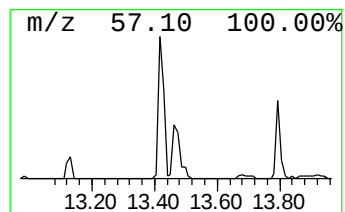
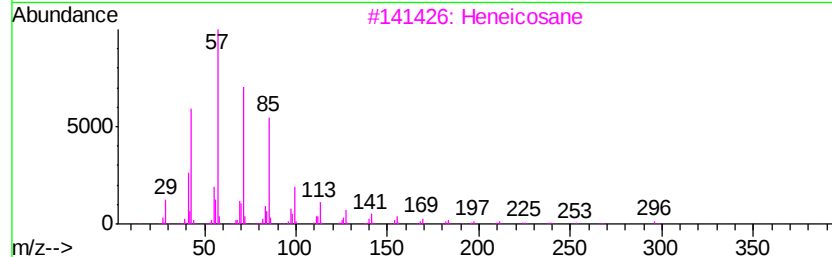
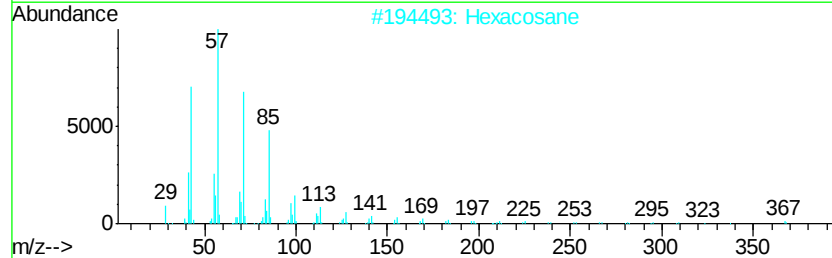
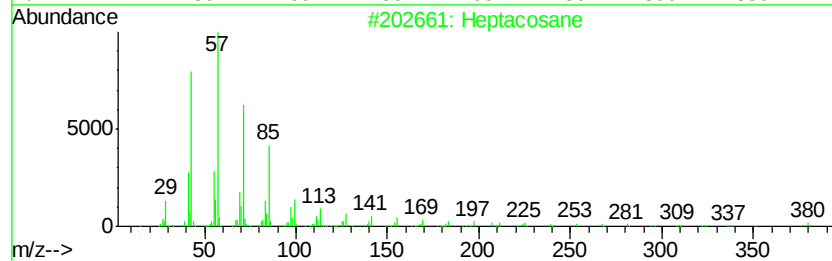
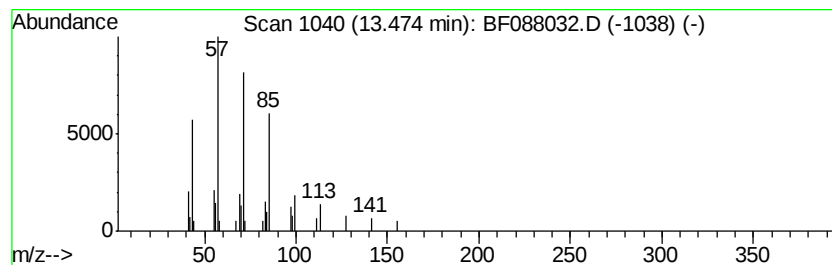
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Heptacosane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	2.20 ng	72572	Chrysene-d12	13.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Octacosane	394	C28H58	000630-02-4	91
5		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061416\
Data File : BF088032.D
Acq On : 15 Jun 2016 7:43
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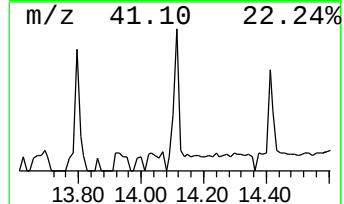
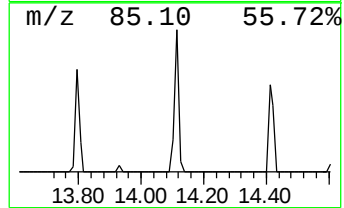
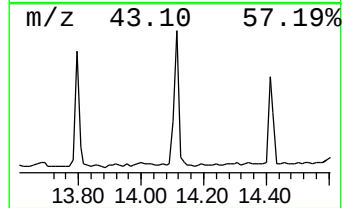
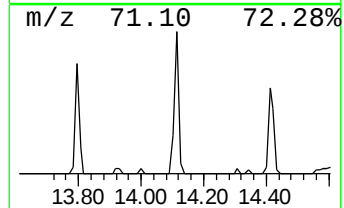
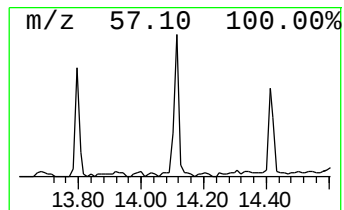
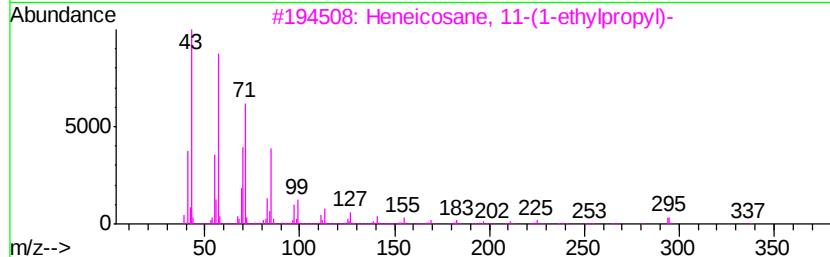
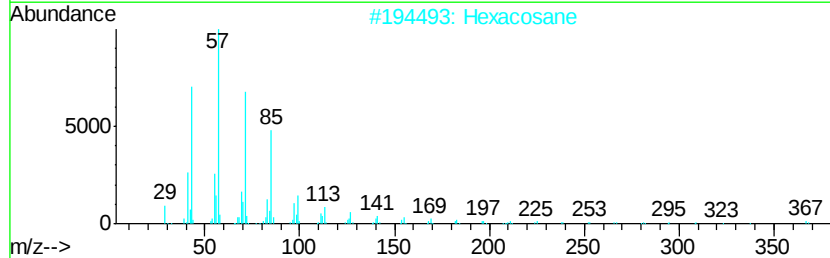
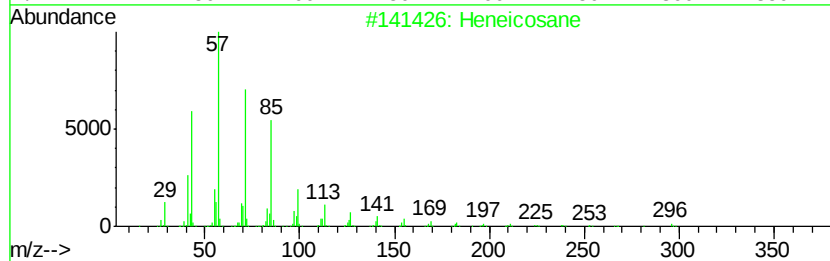
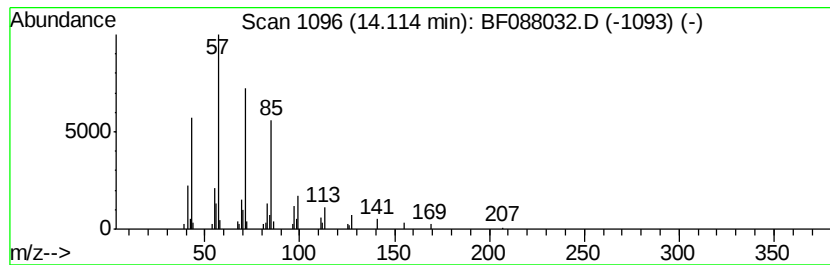
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Heneicosane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.11	2.07 ng	68150	Chrysene-d12	13.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
4		Tetracosane	338	C24H50	000646-31-1	87
5		Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061416\
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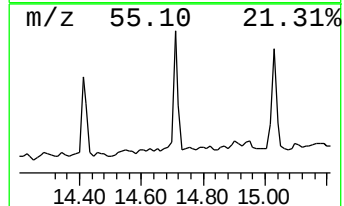
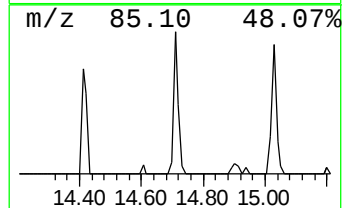
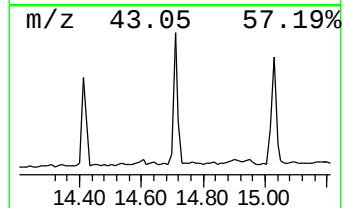
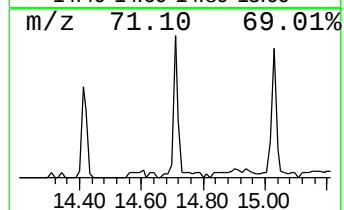
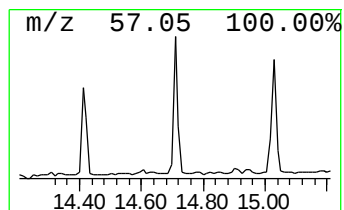
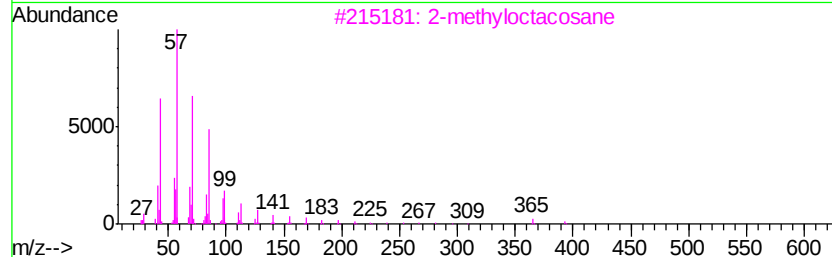
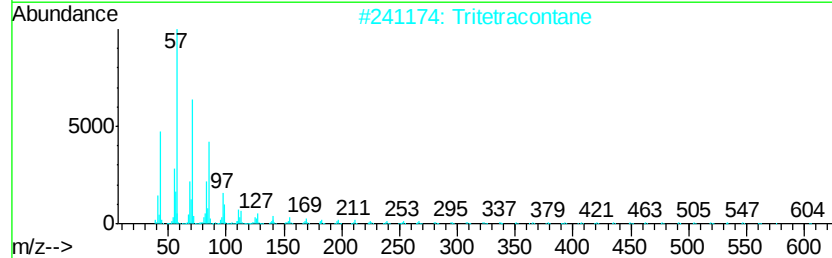
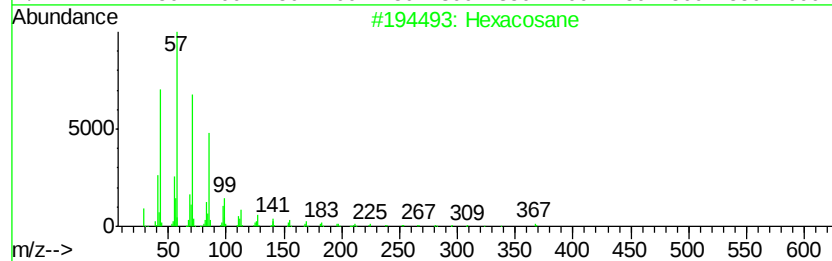
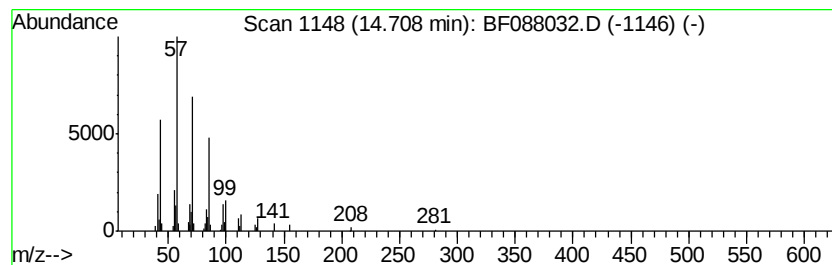
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 Hexacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	3.26 ng	70677	Perylene-d12	15.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Tritetracontane	605	C43H88	007098-21-7	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Heneicosane	296	C21H44	000629-94-7	91
5		Octacosane	394	C28H58	000630-02-4	91



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ALS Vial : 33 Sample Multiplier: 1

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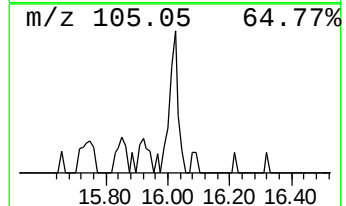
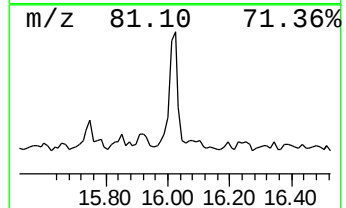
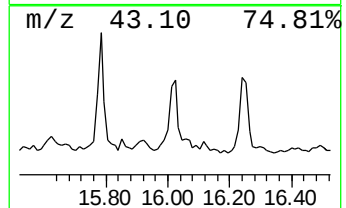
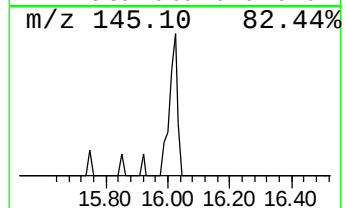
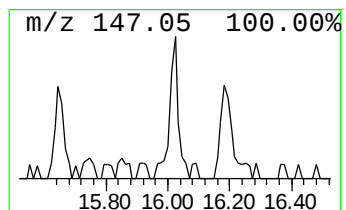
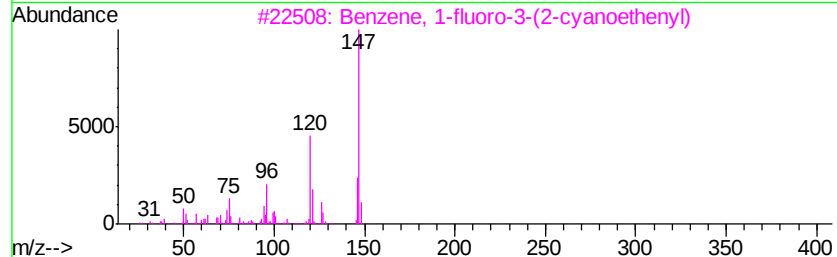
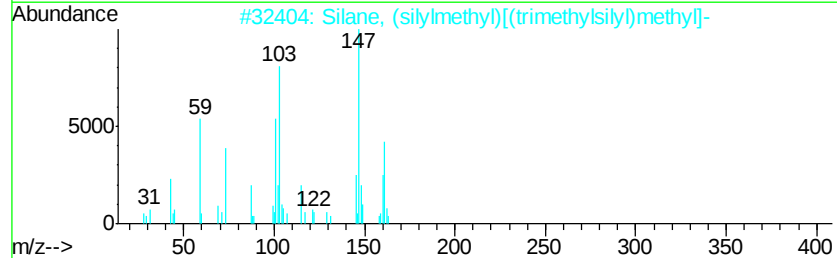
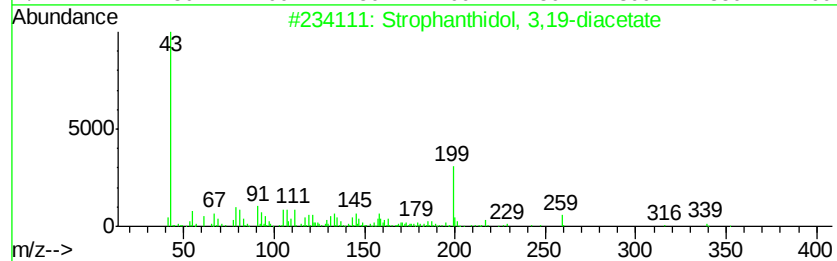
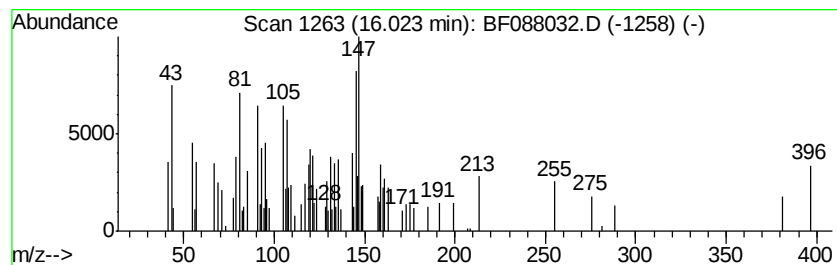
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown16.02 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	4.52 ng	97815	Perylene-d12	15.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Strophanthidol, 3,19-diacetate	490	C27H38O8	083349-11-5	27
2		Silane, (silylmethyl)[(trimethylsilyl)methyl]	162	C5H18Si3	055836-80-1	27
3		Benzene, 1-fluoro-3-(2-cyanoethenyl)	147	C9H6FN	082344-56-7	18
4		Benzene, 1-fluoro-4-(2-cyanoethenyl)	147	C9H6FN	071750-12-4	14
5		Acetic acid 2-oxo-2,3-dihydro-1H-indolizino[1,2-b]pyridine-5-carboxylic acid	218	C11H10N2O3	016780-58-8	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061416\
 Data File : BF088032.D
 Acq On : 15 Jun 2016 7:43
 Operator : UM/SJ
 Sample : H3473-11
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 STA-1100-(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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
n-Propyl acetate	2.55	3.4	ng	98780	1	6.79	583136	20.0
4-Penten-2-one, 4...	3.29	9.1	ng	266004	1	6.79	583136	20.0
3-Hexen-2-one	4.33	218.6	ng	6372390	1	6.79	583136	20.0
2-Pentanone, 4-hy...	4.97	11.1	ng	322898	1	6.79	583136	20.0
unknown6.56	6.56	82.7	ng	2409850	1	6.79	583136	20.0
2-Mercaptobenzoth...	12.02	4.9	ng	171362	4	11.30	699093	20.0
Hexadecanoic acid...	12.72	12.4	ng	409951	5	13.93	658598	20.0
Heptadecyl acetate	12.80	2.4	ng	77637	5	13.93	658598	20.0
Butyl myristate	13.42	7.9	ng	261051	5	13.93	658598	20.0
Heptacosane	13.47	2.2	ng	72572	5	13.93	658598	20.0
Heneicosane	14.11	2.1	ng	68150	5	13.93	658598	20.0
Hexacosane	14.71	3.3	ng	70677	6	15.34	433094	20.0
unknown16.02	16.02	4.5	ng	97815	6	15.34	433094	20.0