

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060816\
 Data File : BF087833.D
 Acq On : 9 Jun 2016 4:46
 Operator : UM/SJ
 Sample : H3405-02
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-13-COMP-0.5-11.0

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-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	1.758	13	15	23	rVB	206517	403577	10.62%	1.533%
2	1.884	24	26	39	rVB	2471347	3800235	100.00%	14.431%
3	2.044	39	40	83	rVB	99573	656300	17.27%	2.492%
4	4.993	296	298	305	rVB	123676	175523	4.62%	0.667%
5	5.416	332	335	338	rVB	1734645	1959087	51.55%	7.440%
6	6.456	423	426	429	rVB	1642857	2019499	53.14%	7.669%
7	6.593	435	438	440	rBV	2307721	2110556	55.54%	8.015%
8	6.822	456	458	461	rBV	580544	561761	14.78%	2.133%
9	6.982	470	472	474	rVB	2001913	1672749	44.02%	6.352%
10	7.393	505	508	510	rBV	1480423	1511164	39.77%	5.739%
11	7.473	513	515	517	rBV	390444	301478	7.93%	1.145%
12	8.113	568	571	573	rBV	887790	765709	20.15%	2.908%
13	9.199	663	666	668	rBV	1885266	2407855	63.36%	9.144%
14	9.588	698	700	702	rBV	232960	186800	4.92%	0.709%
15	9.873	722	725	727	rVB	622875	726344	19.11%	2.758%
16	10.650	791	793	796	rBV2	891631	1309626	34.46%	4.973%
17	10.788	803	805	809	rBV2	28797	49848	1.31%	0.189%
18	11.348	852	854	857	rBV	627115	591963	15.58%	2.248%
19	12.765	976	978	981	rBV	514985	678039	17.84%	2.575%
20	12.936	991	993	996	rBV	1520064	1703969	44.84%	6.471%
21	13.428	1034	1036	1041	rBV	654306	858412	22.59%	3.260%
22	13.508	1041	1043	1045	rBV	258830	300447	7.91%	1.141%
23	13.851	1070	1073	1082	rBV2	62889	101578	2.67%	0.386%
24	13.988	1082	1085	1087	rBV	597358	639623	16.83%	2.429%
25	14.045	1088	1090	1093	rBV	47859	50815	1.34%	0.193%
26	14.114	1093	1096	1099	rBV	25070	49113	1.29%	0.187%
27	14.285	1108	1111	1114	rBV2	76350	91761	2.41%	0.348%
28	14.754	1149	1152	1156	rBV	140677	208175	5.48%	0.791%
29	15.405	1206	1209	1212	rBV	340660	441330	11.61%	1.676%

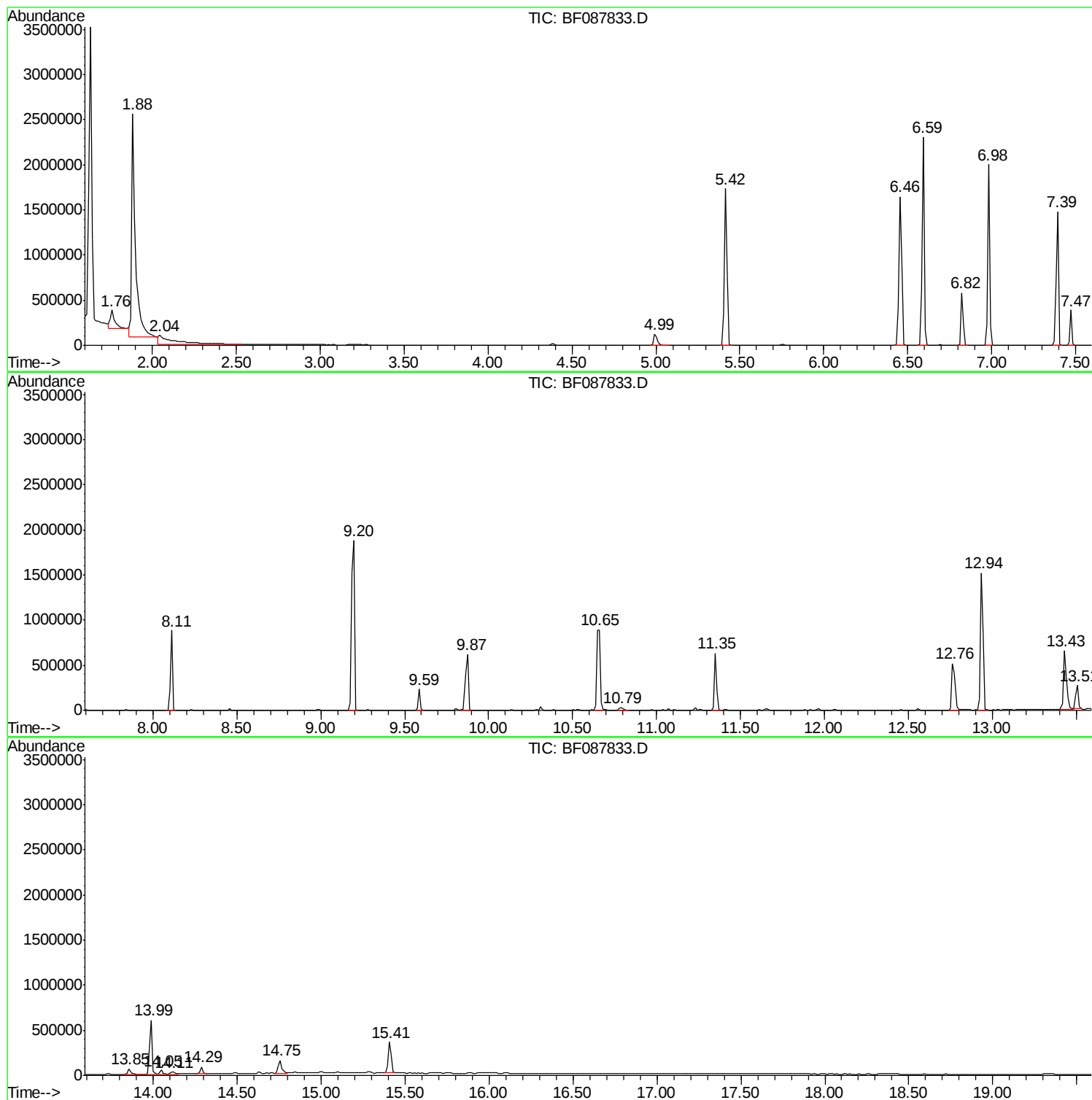
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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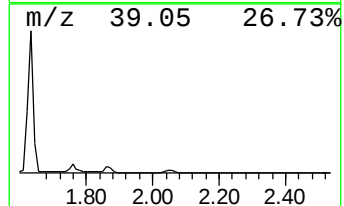
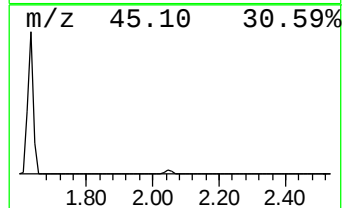
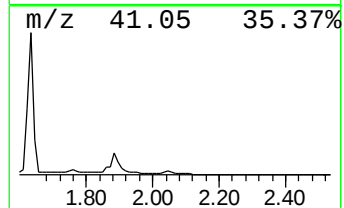
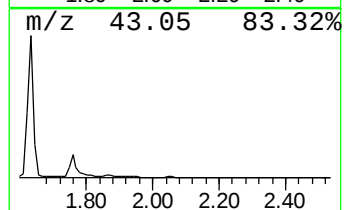
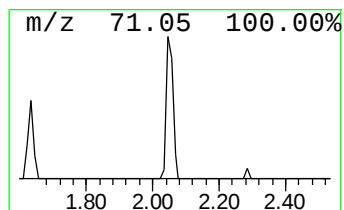
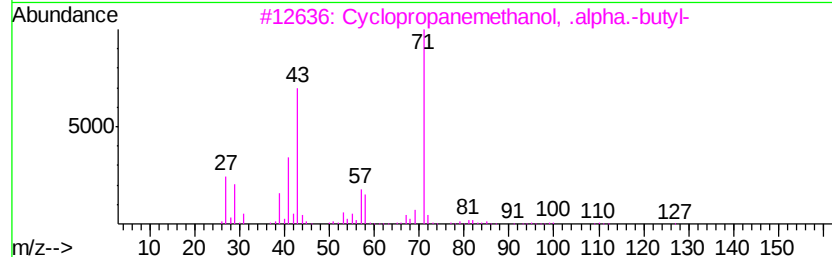
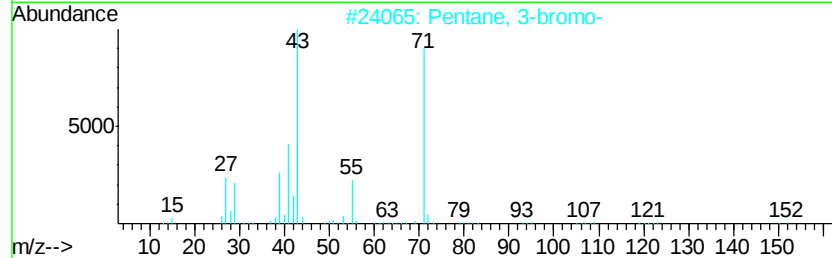
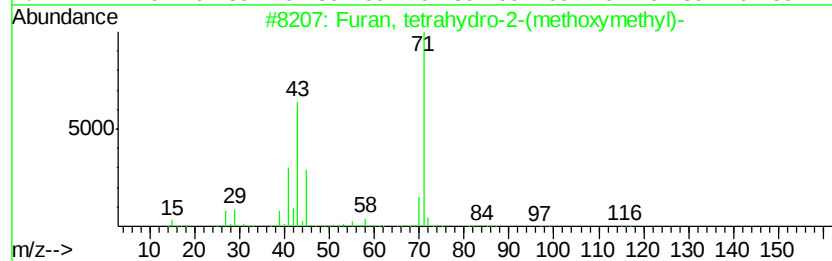
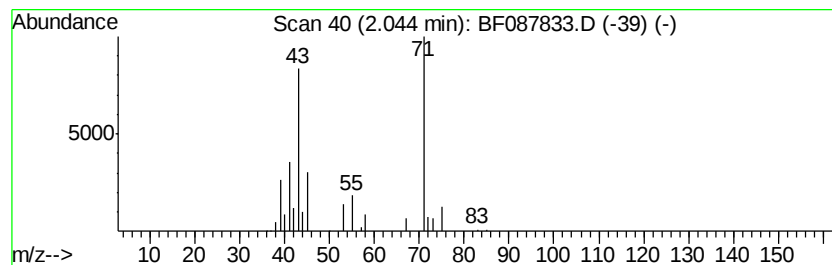
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Furan, tetrahydro-2-(methox... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.04	23.37 ng	656300	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	64
2		Pentane, 3-bromo-	150	C5H11Br	001809-10-5	50
3		Cyclopropanemethanol, .alpha.-bu...	128	C8H16O	004379-16-2	39
4		Pantolactone	130	C6H10O3	000599-04-2	38
5		2-Furanmethanol, tetrahydro-	102	C5H10O2	000097-99-4	38



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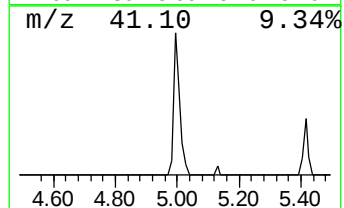
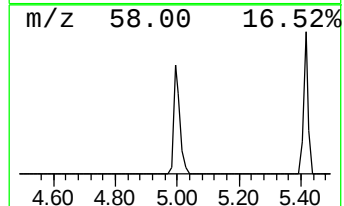
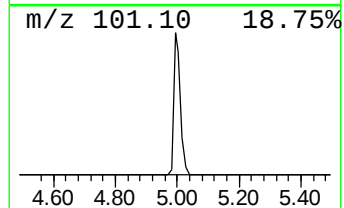
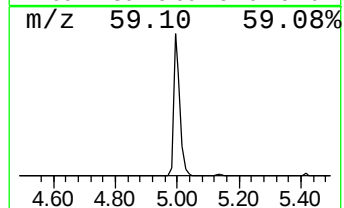
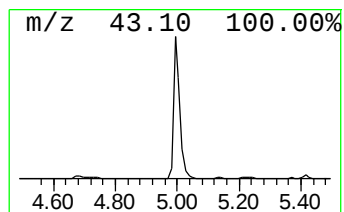
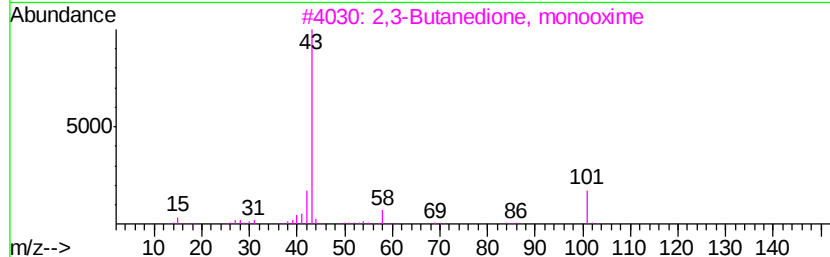
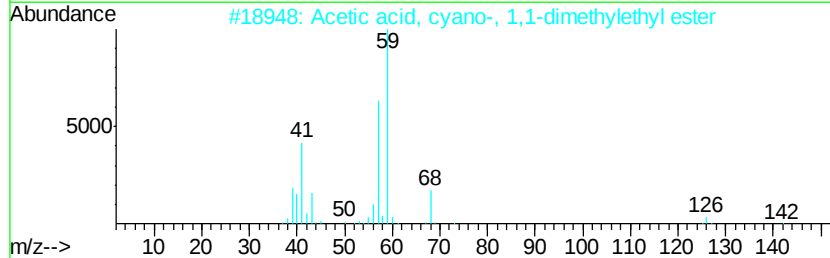
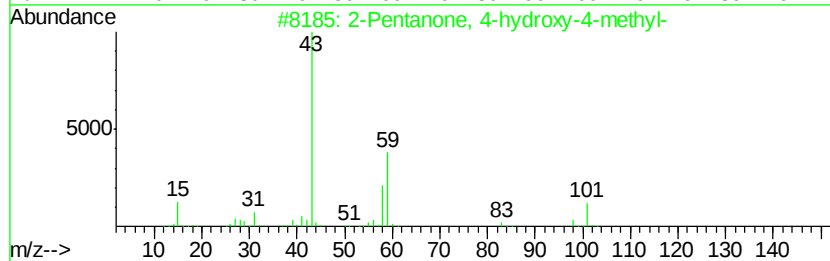
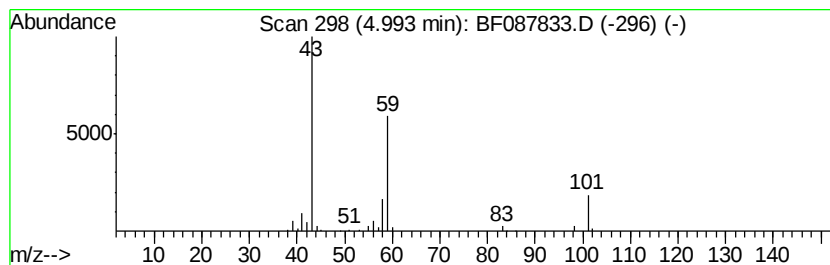
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	6.25 ng	175523	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	59
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9



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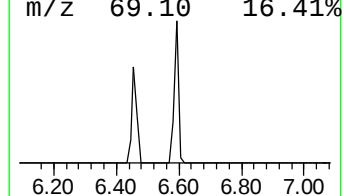
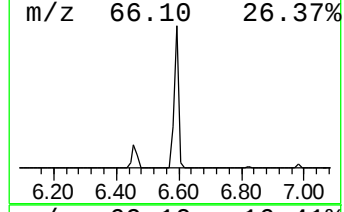
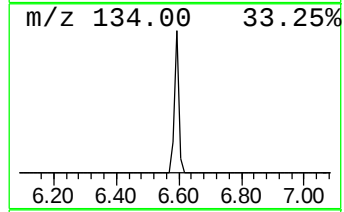
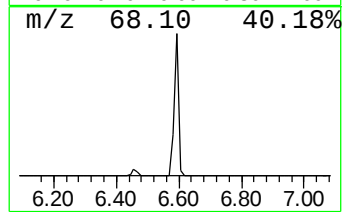
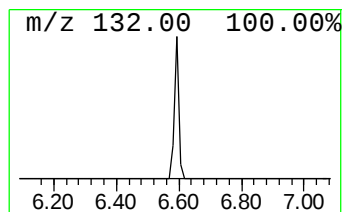
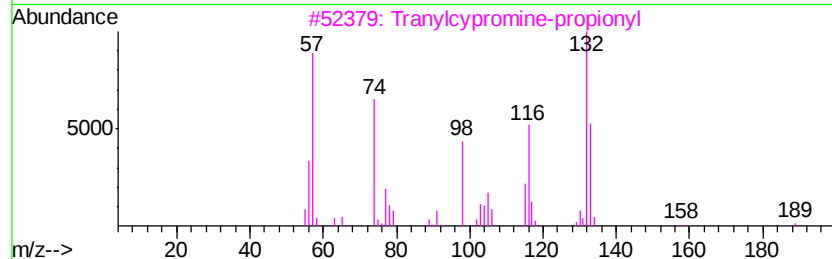
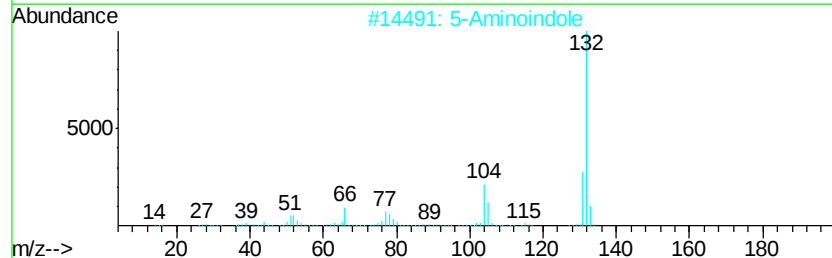
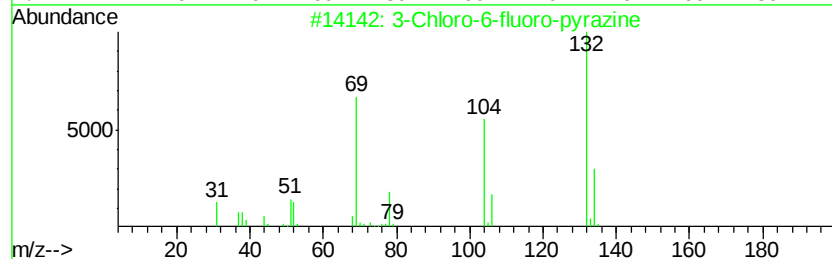
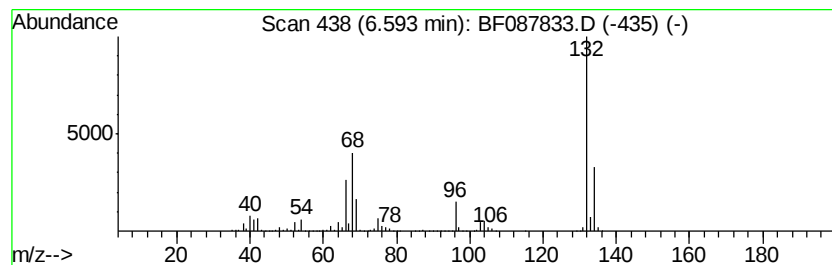
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Peak Number 5 unknown6.59 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	75.14 ng	2110560	1,4-Dichlorobenzene-d4	6.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole			132	C8H8N2	005192-03-0	12
3	Tranvlcvpromine-propionyl			189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...			132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine			132	C4H2ClFN2	051422-00-5	9



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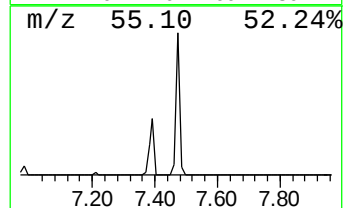
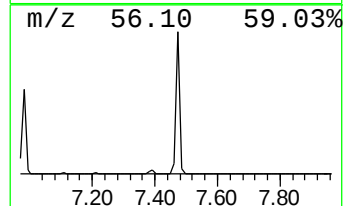
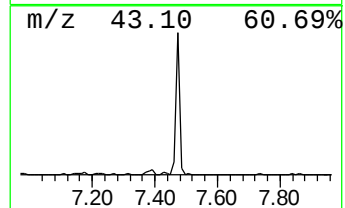
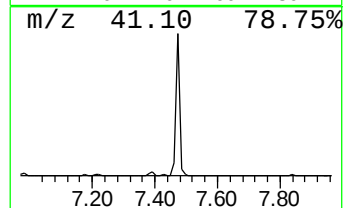
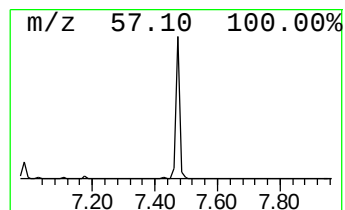
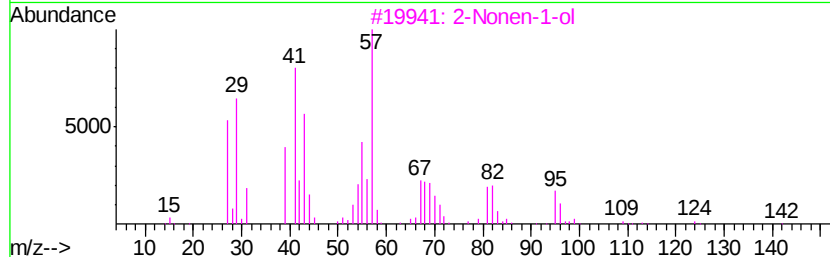
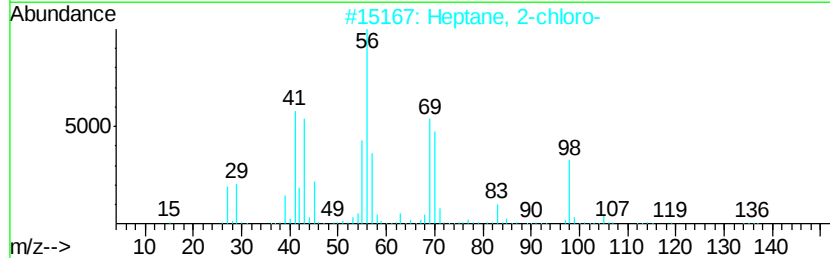
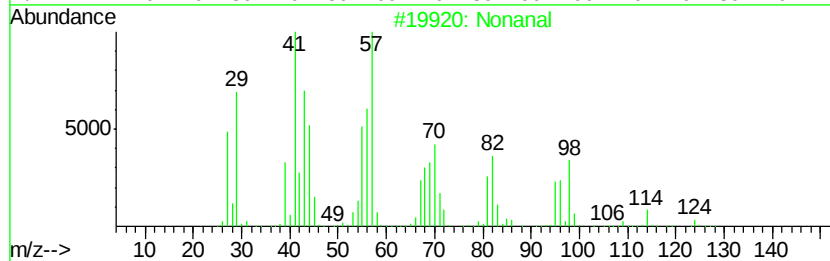
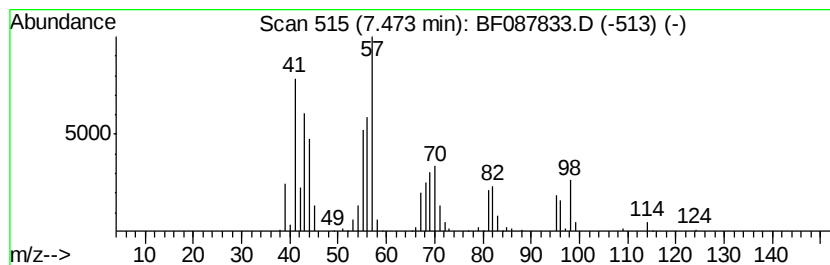
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Peak Number 7 Nonanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.47	7.87 ng	301478	Naphthalene-d8	8.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonanal	142	C9H18O	000124-19-6	91
2		Heptane, 2-chloro-	134	C7H15Cl	001001-89-4	27
3		2-Nonen-1-ol	142	C9H18O	022104-79-6	27
4		5-Methyl-2-hexene, c&t	98	C7H14	003404-62-4	27
5		(Z)-Hex-2-ene, 5-methyl-	98	C7H14	013151-17-2	27



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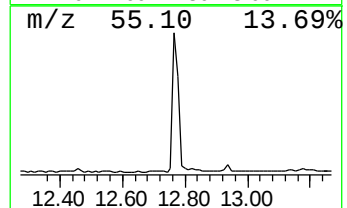
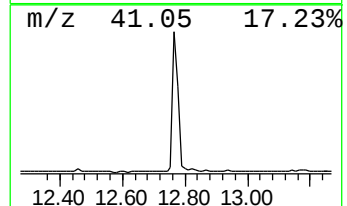
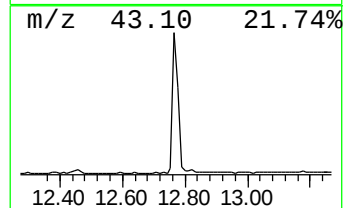
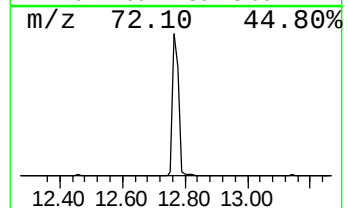
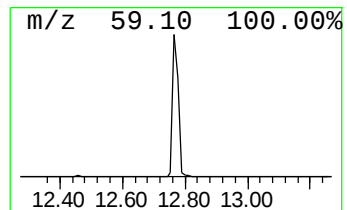
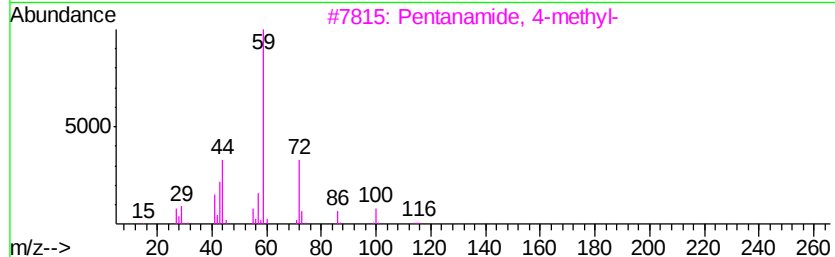
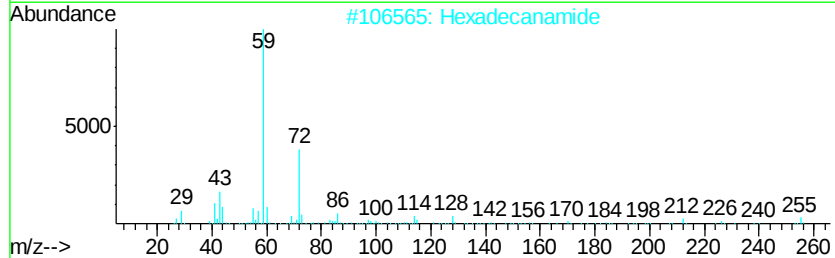
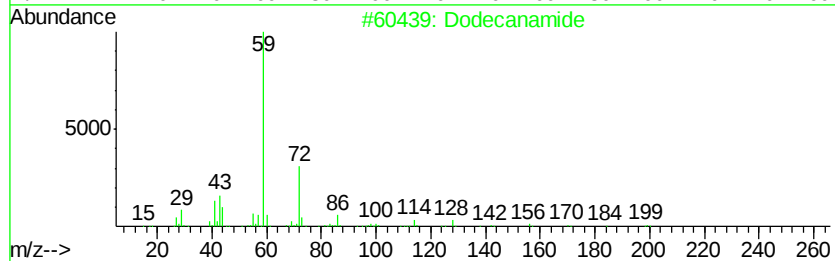
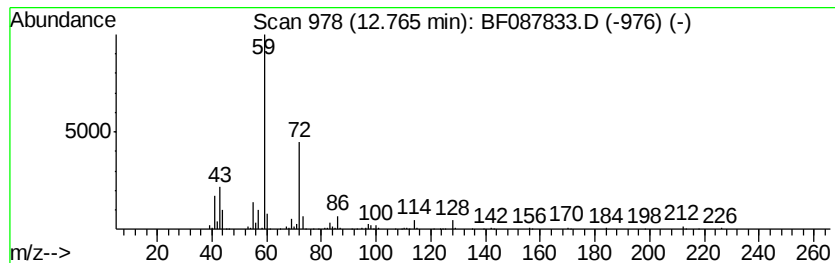
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Peak Number 8 Dodecanamide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	21.20 ng	678039	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecanamide	199	C12H25NO	001120-16-7	90
2		Hexadecanamide	255	C16H33NO	000629-54-9	87
3		Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	64
4		Tetradecanamide	227	C14H29NO	000638-58-4	64
5		Undecanamide, 11-bromo-	263	C11H22BrNO	005875-26-3	64



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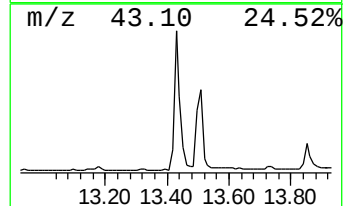
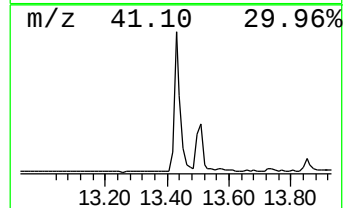
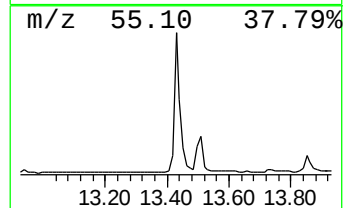
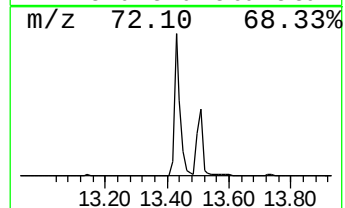
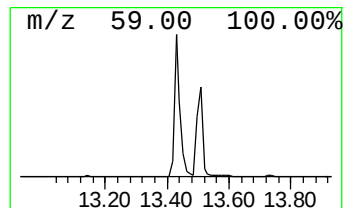
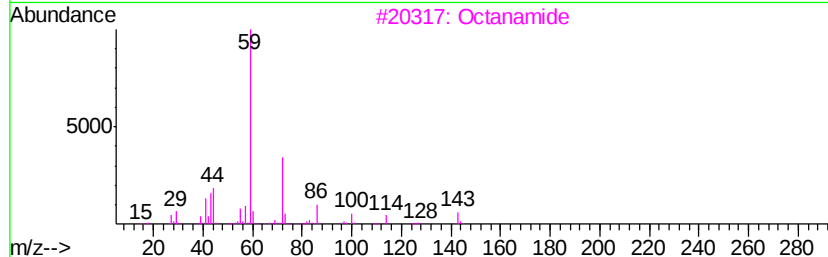
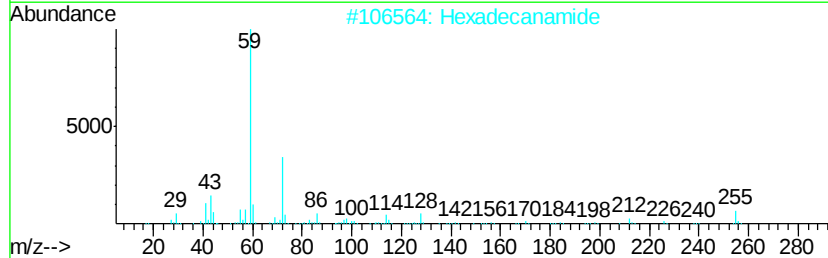
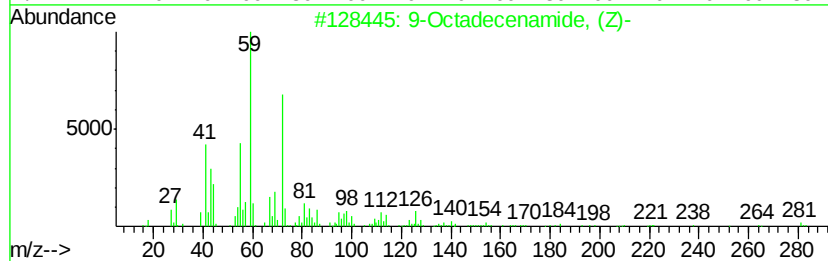
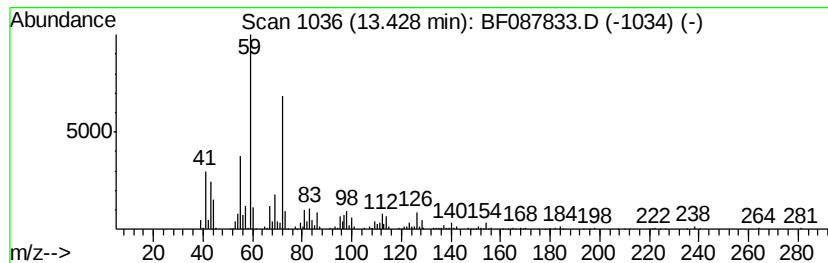
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.43	26.84 ng	858412	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2		Hexadecanamide	255	C16H33NO	000629-54-9	78
3		Octanamide	143	C8H17NO	000629-01-6	59
4		Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	56
5		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	50



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060816\
Data File : BF087833.D
Acq On : 9 Jun 2016 4:46
Operator : UM/SJ
Sample : H3405-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-13-COMP-0.5-11.0

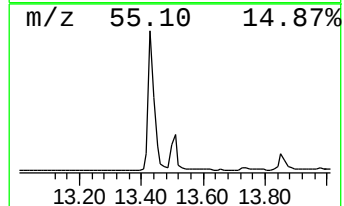
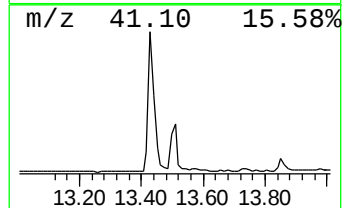
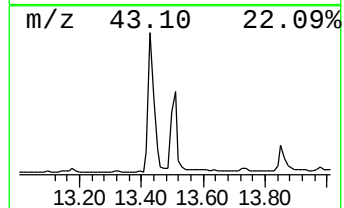
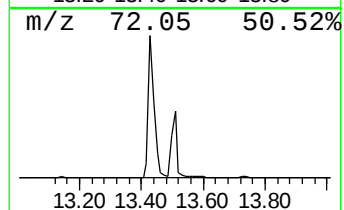
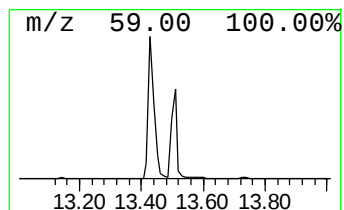
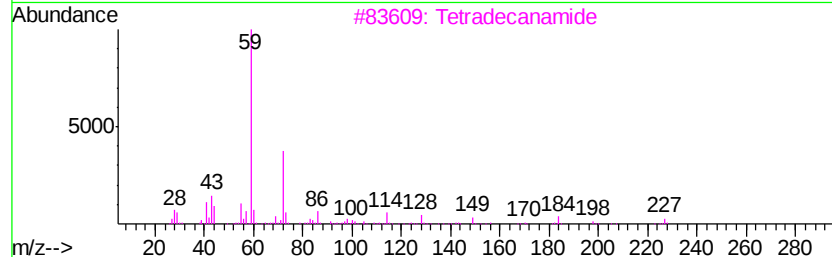
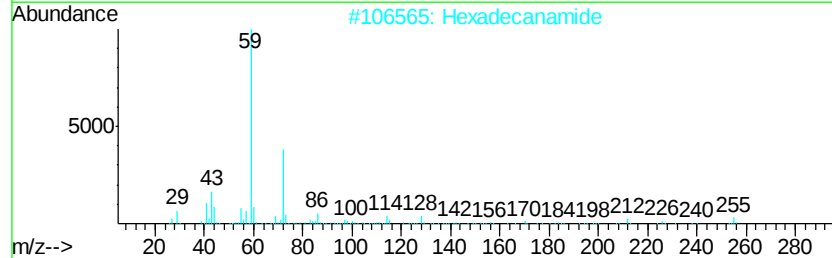
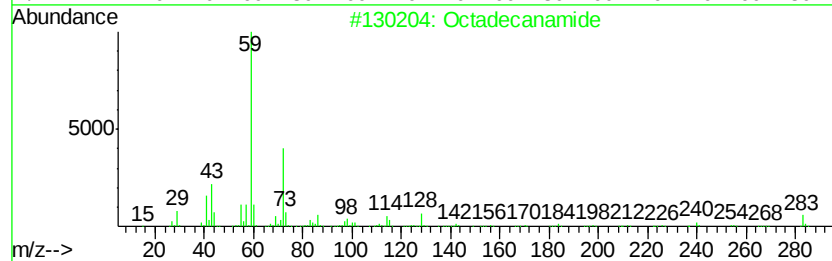
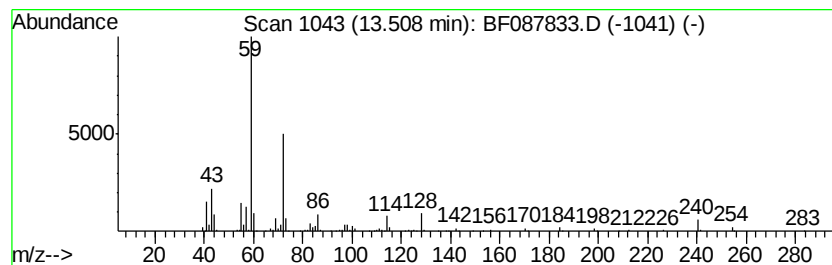
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecanamide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.51	9.39 ng	300447	Chrysene-d12	13.99

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanamide	283	C18H37NO	000124-26-5	91
2			Hexadecanamide	255	C16H33NO	000629-54-9	86
3			Tetradecanamide	227	C14H29NO	000638-58-4	86
4			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	78
5			Decanamide-	171	C10H21NO	002319-29-1	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060816\
Data File : BF087833.D
Acq On : 9 Jun 2016 4:46
Operator : UM/SJ
Sample : H3405-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

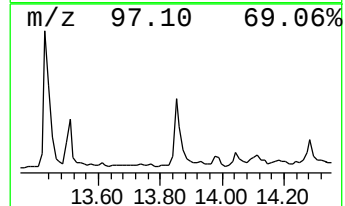
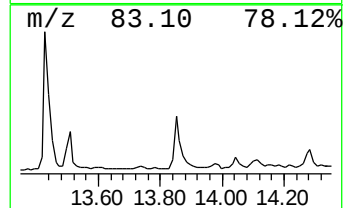
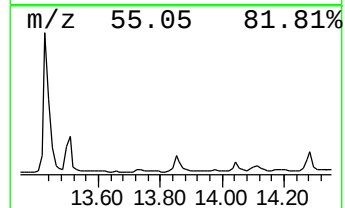
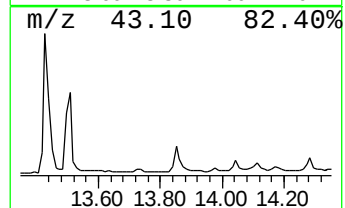
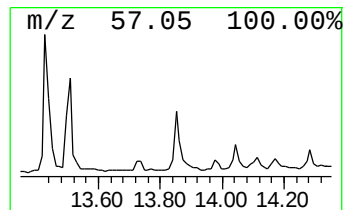
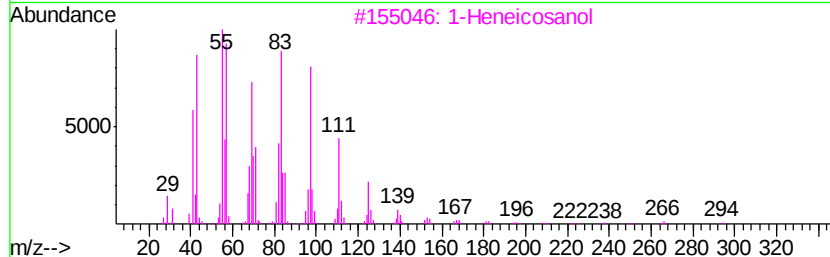
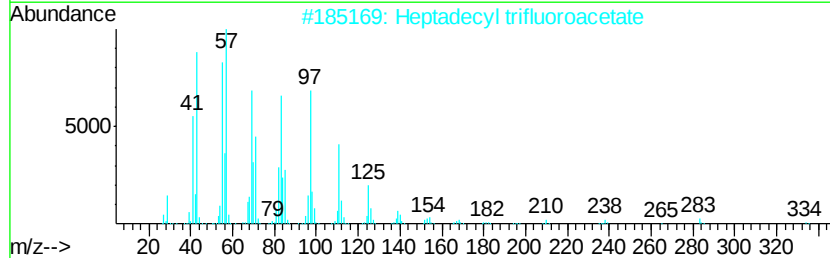
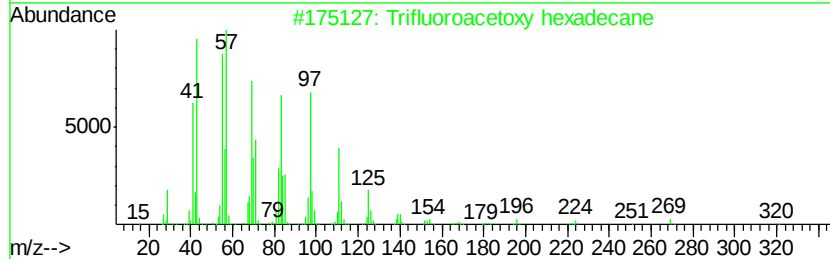
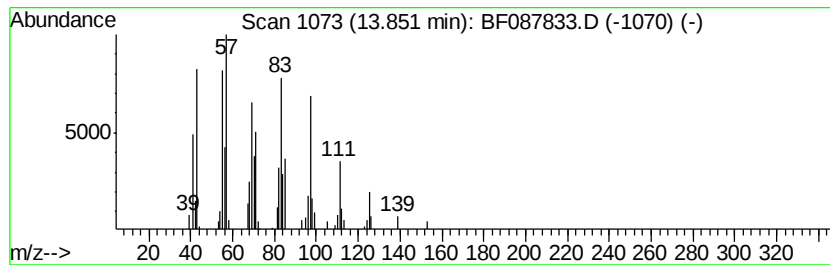
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Trifluoroacetoxy hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.85	3.18 ng	101578	Chrysene-d12	13.99	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060816\
Data File : BF087833.D
Acq On : 9 Jun 2016 4:46
Operator : UM/SJ
Sample : H3405-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-13-COMP-0.5-11.0

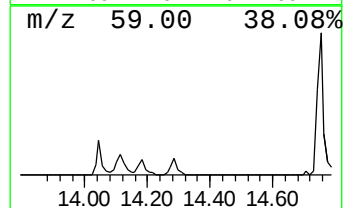
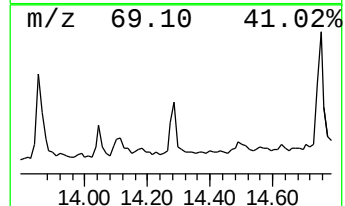
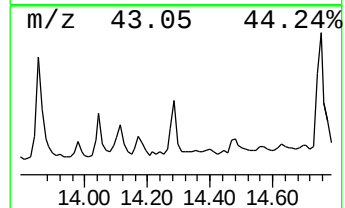
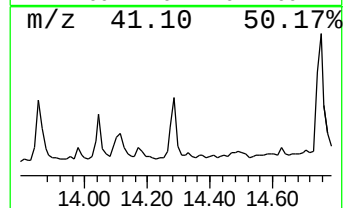
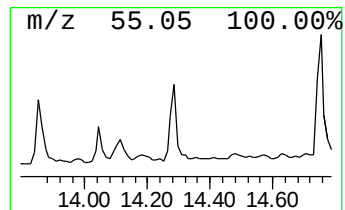
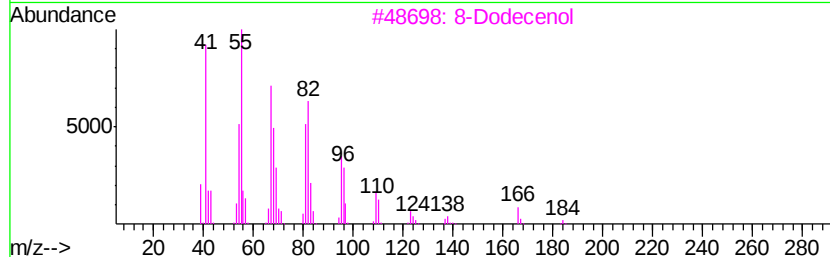
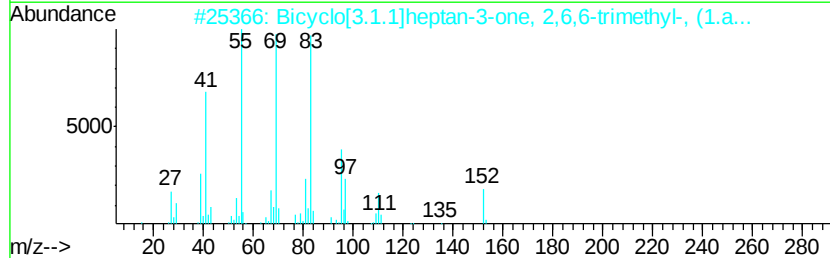
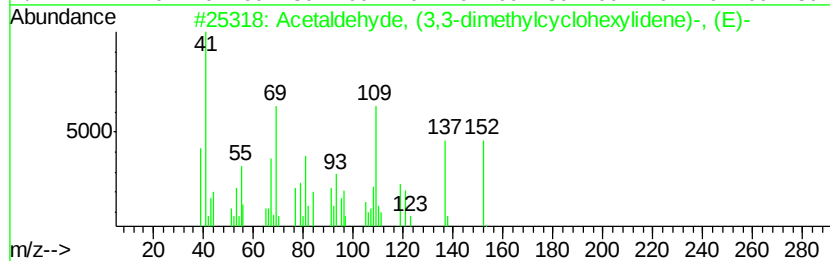
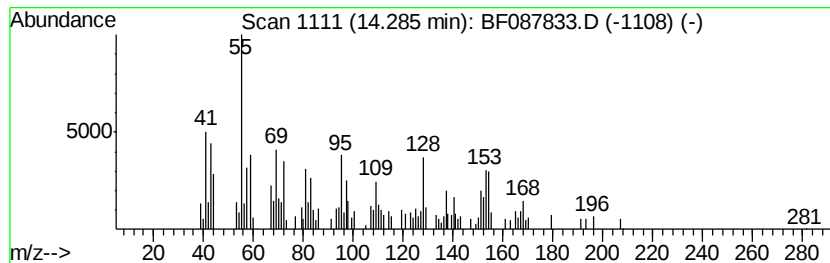
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown14.29 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.29	2.87 ng	91761	Chrysene-d12	13.99

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde, (3,3-dimethylcyclo...	152	C10H16O	026532-25-2	25
2			Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	15
3			8-Dodecenol	184	C12H24O	042513-42-8	14
4			Z,Z-4,16-Octadecadien-1-ol acetate	308	C20H36O2	1000130-95-7	14
5			2-Pentenoic acid, 4-methyl-, met...	128	C7H12O2	050652-78-3	11



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Sample : H3405-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-13-COMP-0.5-11.0

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
Furan, tetrahydro...	2.04	23.4	ng	656300	1	6.82	561761	20.0
2-Pentanone, 4-hy...	4.99	6.3	ng	175523	1	6.82	561761	20.0
unknown6.59	6.59	75.1	ng	2110560	1	6.82	561761	20.0
Nonanal	7.47	7.9	ng	301478	2	8.11	765709	20.0
Dodecanamide	12.77	21.2	ng	678039	5	13.99	639623	20.0
9-Octadecenamide, ...	13.43	26.8	ng	858412	5	13.99	639623	20.0
Octadecanamide	13.51	9.4	ng	300447	5	13.99	639623	20.0
Trifluoroacetoxy ...	13.85	3.2	ng	101578	5	13.99	639623	20.0
unknown14.29	14.29	2.9	ng	91761	5	13.99	639623	20.0