

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
 Data File : BF086784.D
 Acq On : 7 May 2016 20:04
 Operator : UM/SJ
 Sample : H2878-05
 Misc :
 ALS Vial : 54 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 URSMW-14

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-BF050416.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	4.876	242	244	252	rBV	98862	206398	2.95%	0.443%
2	5.299	279	281	284	rBV	2424765	3258067	46.54%	6.998%
3	6.350	371	373	376	rBV	1585810	2348822	33.55%	5.045%
4	6.476	382	384	386	rBV	5281034	5363988	76.61%	11.521%
5	6.704	401	404	409	rBV	998788	1205596	17.22%	2.589%
6	6.853	415	417	420	rBV	3488750	4696113	67.07%	10.086%
7	6.979	425	428	432	rVB	42865	74632	1.07%	0.160%
8	7.276	451	454	456	rBV	3778097	4250204	60.71%	9.129%
9	7.985	514	516	519	rBV	1354641	1486930	21.24%	3.194%
10	8.956	598	601	604	rBV	45301	71085	1.02%	0.153%
11	9.070	607	611	613	rBV	6118735	7001324	100.00%	15.038%
12	9.470	643	646	647	rBV	67494	77033	1.10%	0.165%
13	9.676	660	664	667	rBV2	77373	106646	1.52%	0.229%
14	9.733	667	669	672	rBV	1506486	1594436	22.77%	3.425%
15	10.179	703	708	709	rBV2	102571	122163	1.74%	0.262%
16	10.396	724	727	730	rBV	37590	73452	1.05%	0.158%
17	10.533	735	739	741	rBV2	2920306	4251123	60.72%	9.131%
18	10.648	746	749	753	rVB	118266	156776	2.24%	0.337%
19	11.219	796	799	801	rBV	1317444	1494050	21.34%	3.209%
20	11.436	816	818	820	rBV	90560	108116	1.54%	0.232%
21	11.756	844	846	853	rBV2	143287	215298	3.08%	0.462%
22	12.545	913	915	917	rBV	88990	141126	2.02%	0.303%
23	12.591	917	919	921	rVV	140651	161656	2.31%	0.347%
24	12.625	921	922	925	rVB	213608	252256	3.60%	0.542%
25	12.808	935	938	940	rBV	3845582	5236253	74.79%	11.247%
26	13.334	981	984	986	rBV	204094	186446	2.66%	0.400%
27	13.379	986	988	989	rVV	50848	70423	1.01%	0.151%
28	13.585	1003	1006	1012	rBV3	62607	119240	1.70%	0.256%
29	13.711	1014	1017	1024	rBV	184884	248574	3.55%	0.534%
30	13.837	1026	1028	1031	rBV	763173	1087437	15.53%	2.336%
31	15.220	1146	1149	1157	rBV	679332	893266	12.76%	1.919%

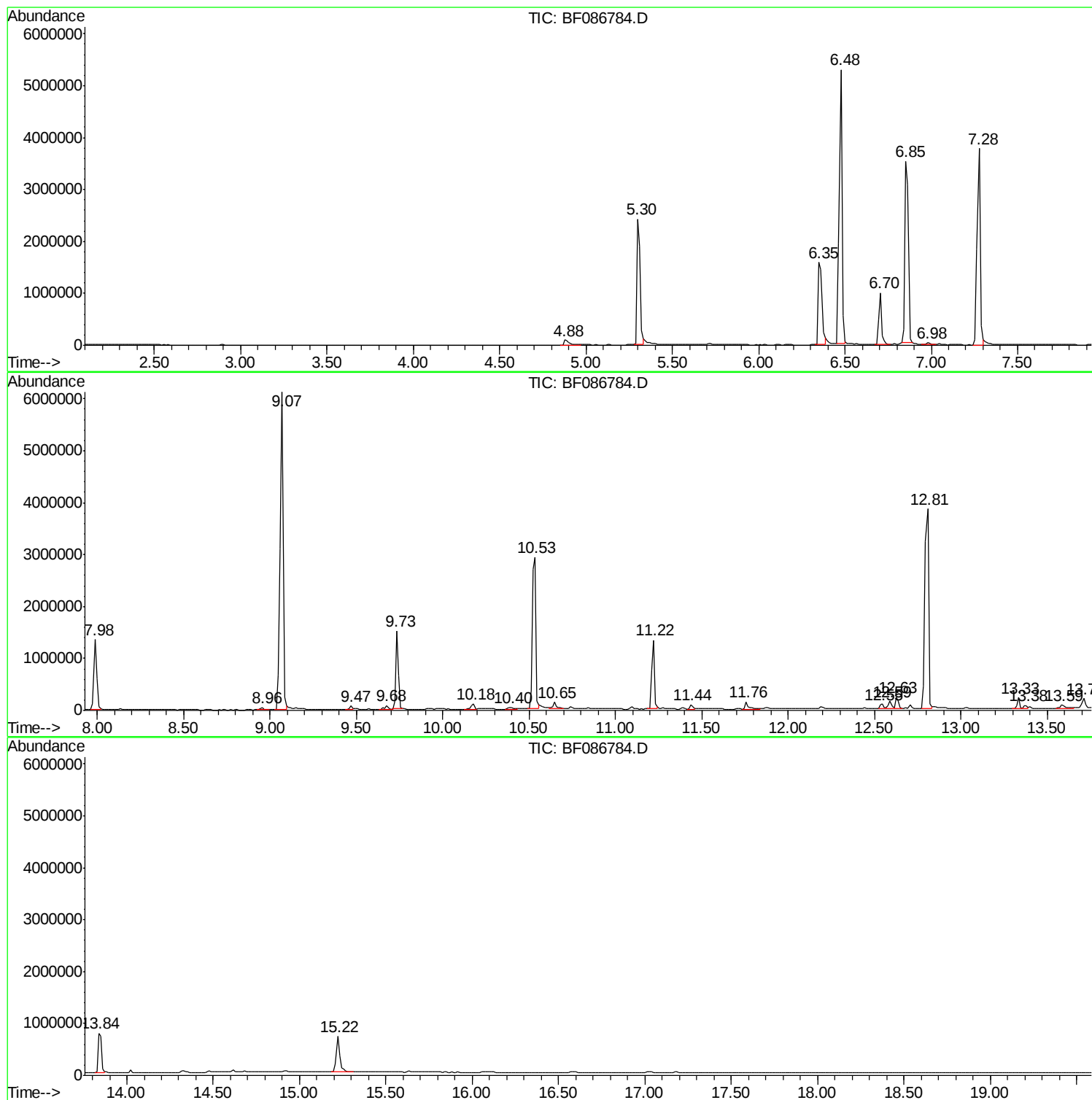
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Misc :
ALS Vial : 54 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
URSMW-14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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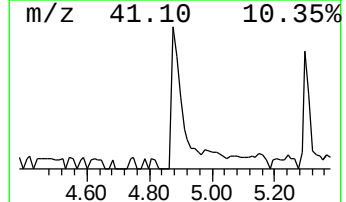
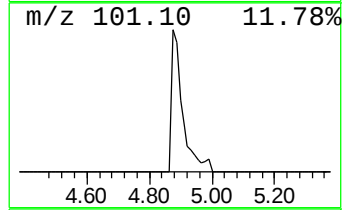
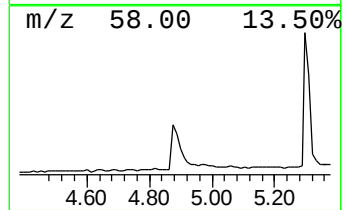
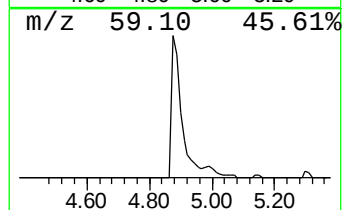
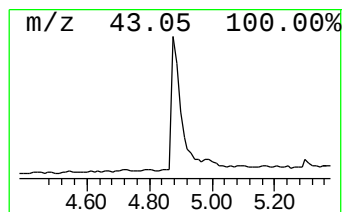
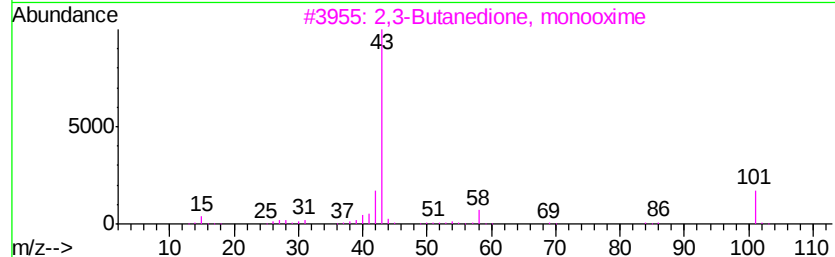
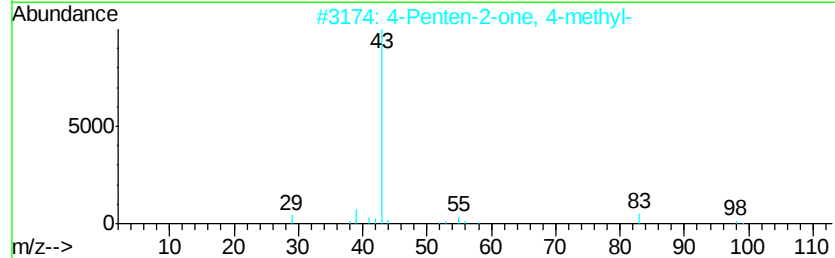
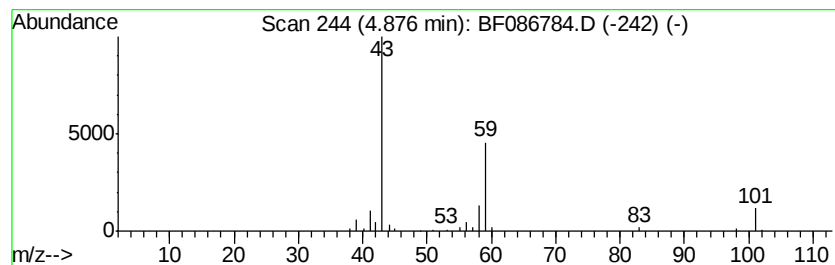
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	6.85 ng	206398	1,4-Dichlorobenzene-d4	6.70

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Diacetamide	101	C4H7NO2	000625-77-4	9
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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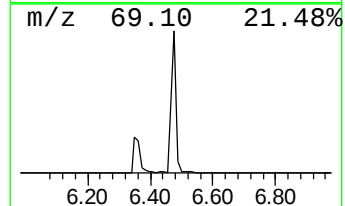
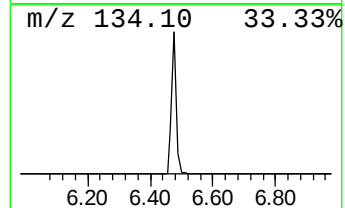
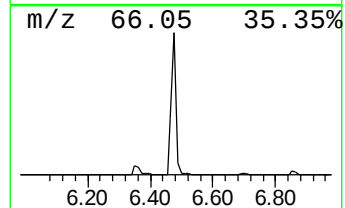
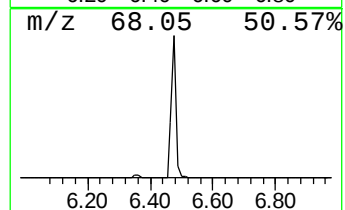
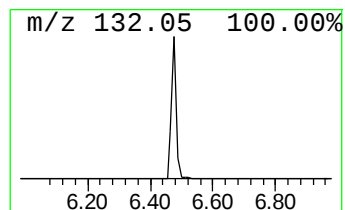
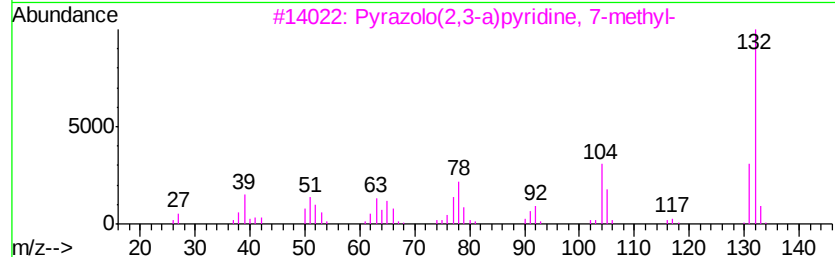
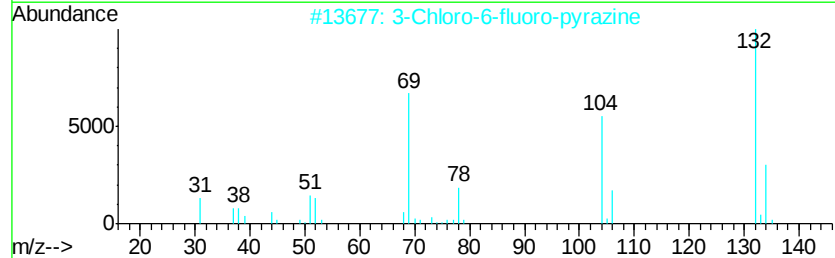
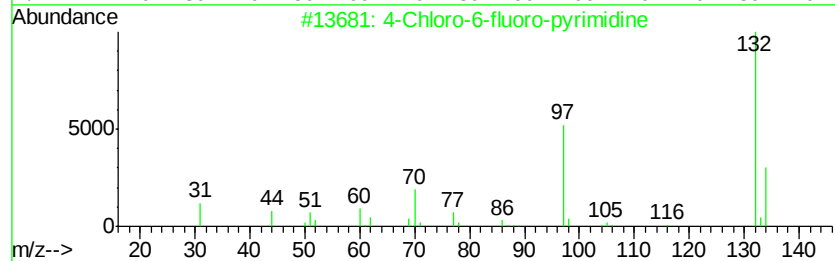
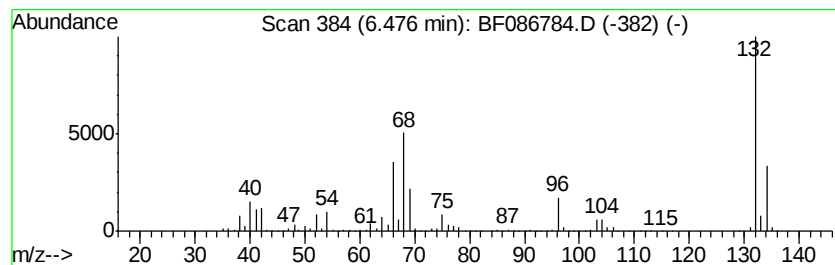
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Peak Number 2 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	177.97 ng	5363990	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	22
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22



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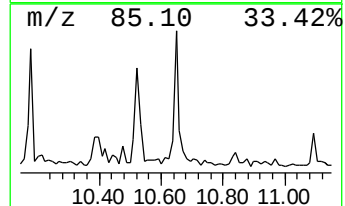
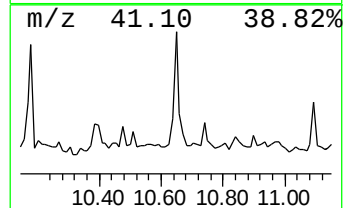
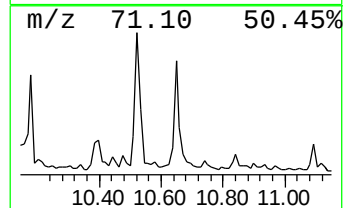
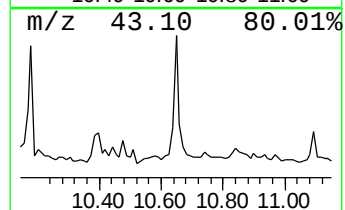
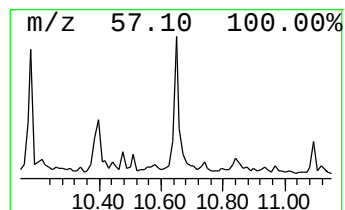
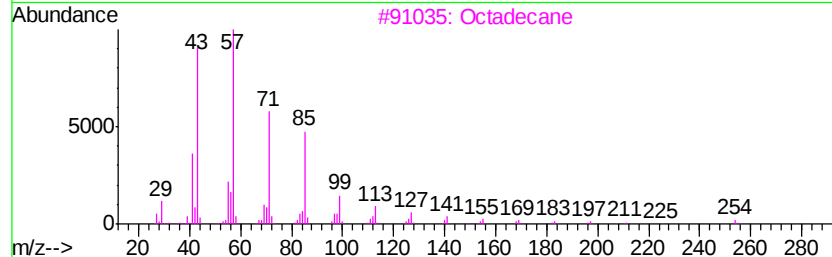
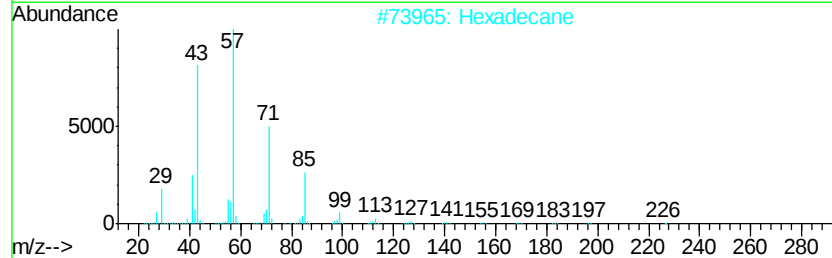
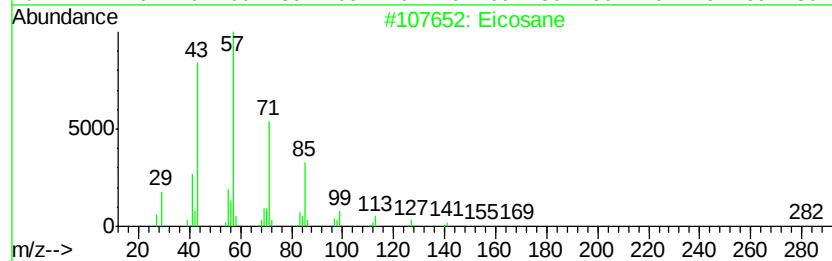
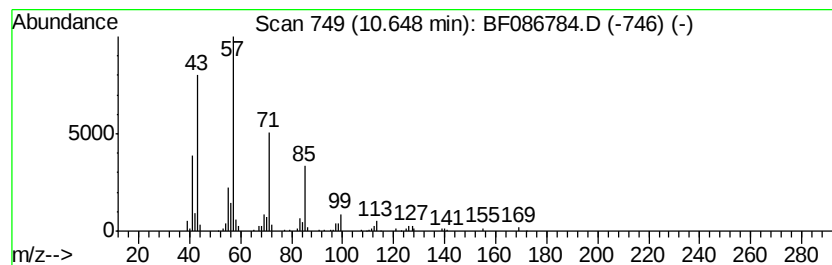
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	4.20 ng	156776	Phenanthrene-d10	11.22

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Hexadecane		226	C16H34	000544-76-3	91
3	Octadecane		254	C18H38	000593-45-3	90
4	Pentadecane		212	C15H32	000629-62-9	86
5	Heptadecane		240	C17H36	000629-78-7	80



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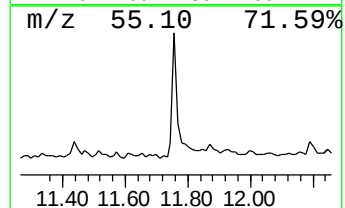
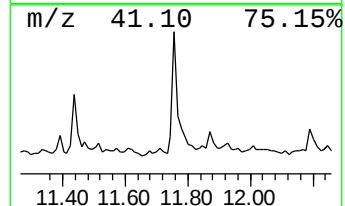
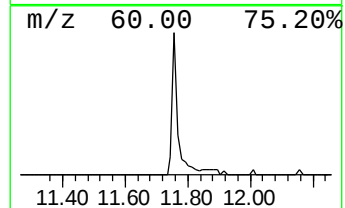
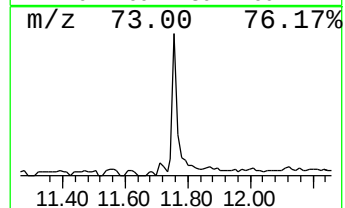
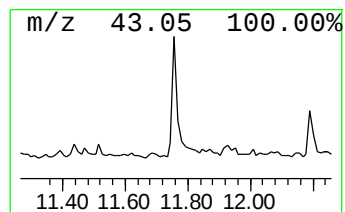
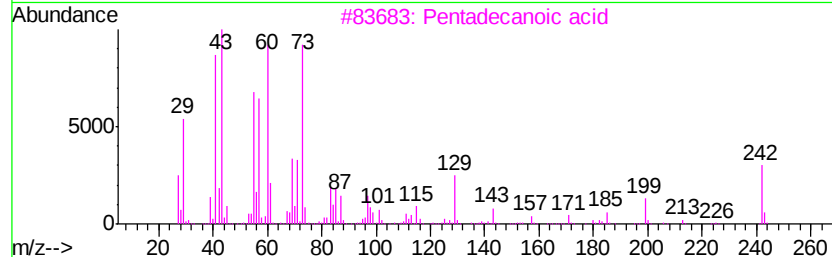
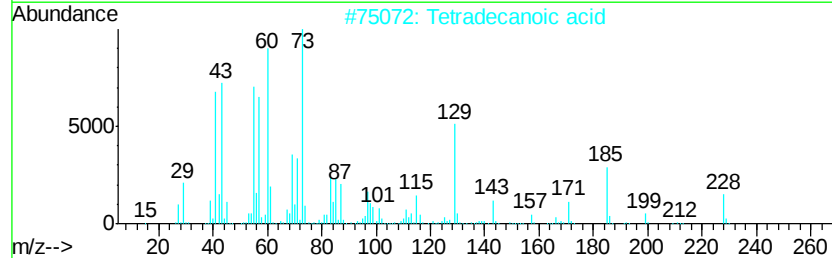
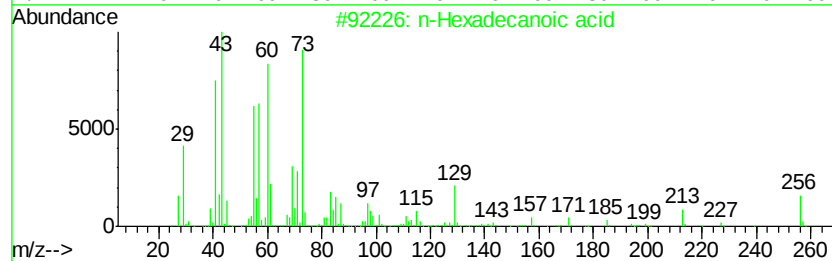
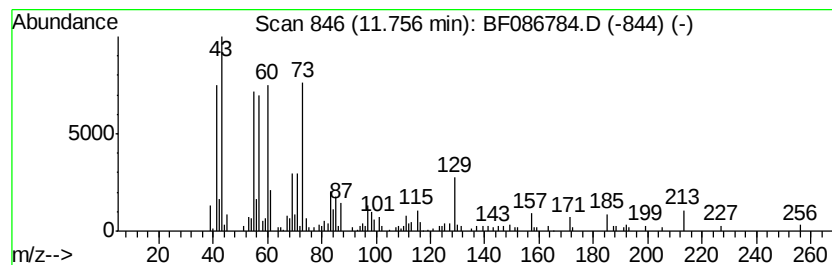
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.76	5.76 ng	215298	Phenanthrene-d10	11.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4		Tridecanoic acid	214	C13H26O2	000638-53-9	80
5		Undecanoic acid	186	C11H22O2	000112-37-8	72



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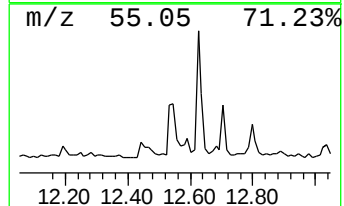
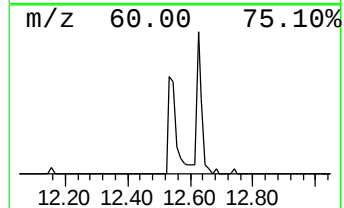
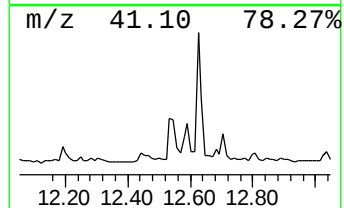
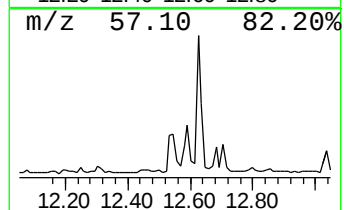
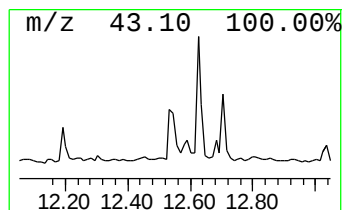
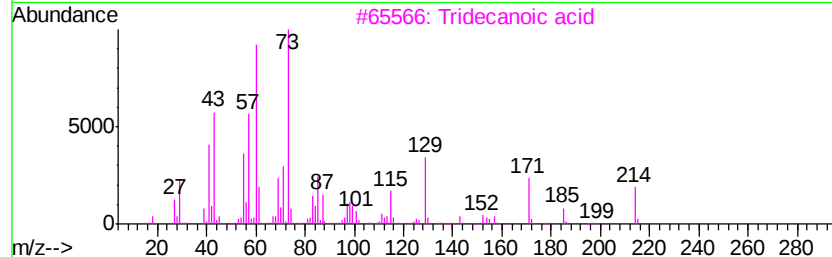
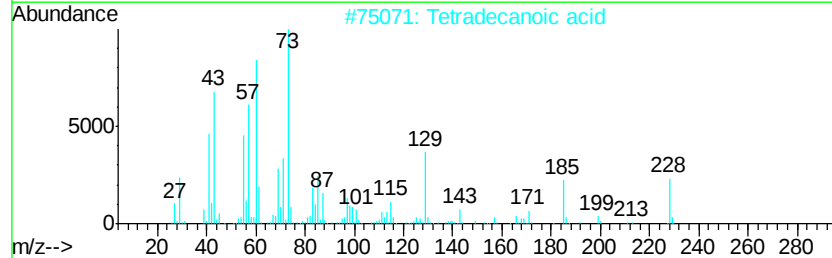
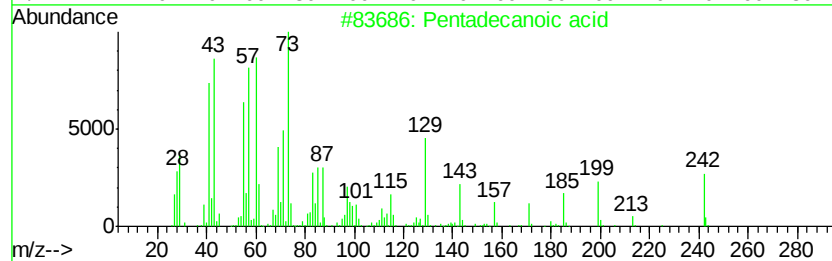
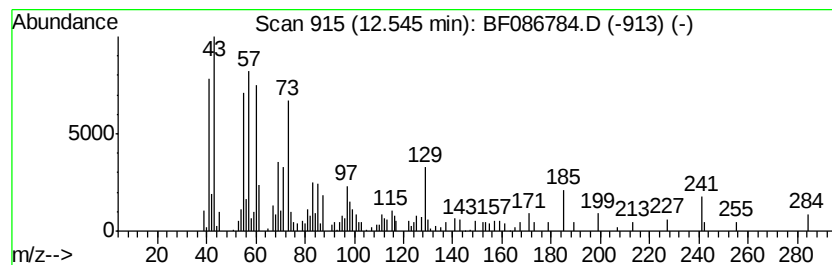
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Peak Number 6 Pentadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.55	5.19 ng	141126	Chrysene-d12	13.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecanoic acid	242	C15H30O2	001002-84-2	59
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	58
3		Tridecanoic acid	214	C13H26O2	000638-53-9	53
4		Dodecanoic acid	200	C12H24O2	000143-07-7	47
5		Undecanoic acid	186	C11H22O2	000112-37-8	43



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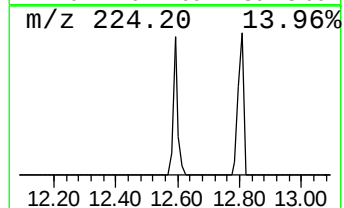
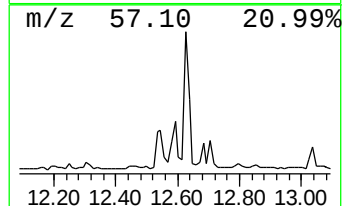
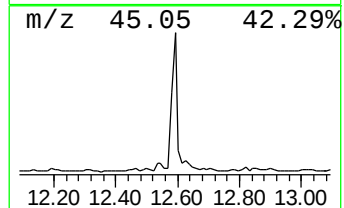
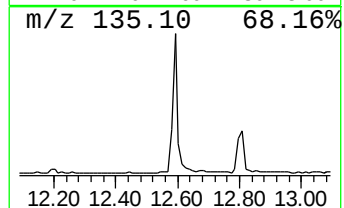
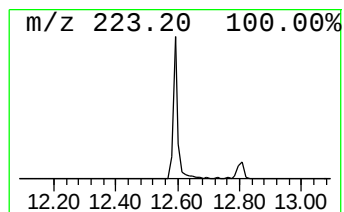
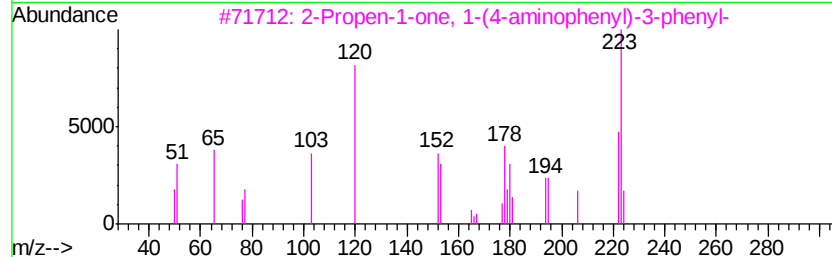
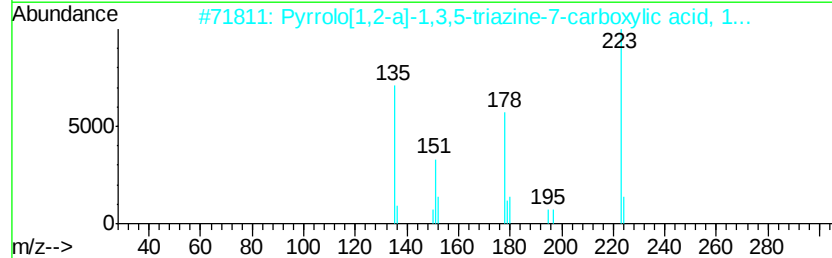
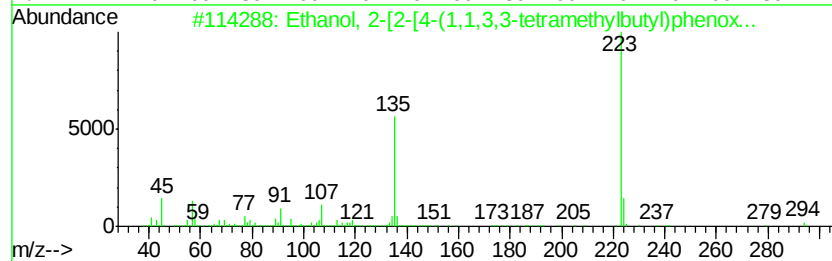
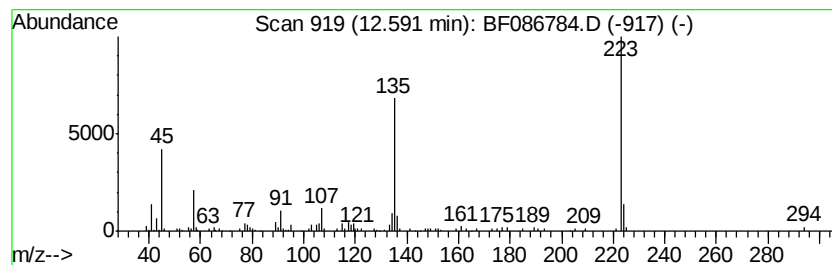
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Ethanol, 2-[2-[4-(1,1,3,3-t... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.59	5.95 ng	161656	Chrysene-d12		13.85	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	97	
2	Pyrrolo[1,2-a]-1,3,5-triazine-7-...	223	C9H9N3O4	054449-89-7	83	
3	2-Propen-1-one, 1-(4-aminophenyl...	223	C15H13NO	002403-30-7	43	
4	1H-Benzimidazole, 2-(5-ethyl-2-p...	223	C14H13N3	067273-43-2	35	
5	Phenol, 4,4'-(1,2-diethyl-1,2-et...	270	C18H22O2	000084-16-2	22	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
Data File : BF086784.D
Acq On : 7 May 2016 20:04
Operator : UM/SJ
Sample : H2878-05
Misc :
ALS Vial : 54 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
URSMW-14

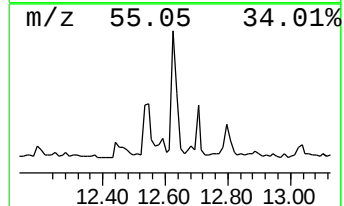
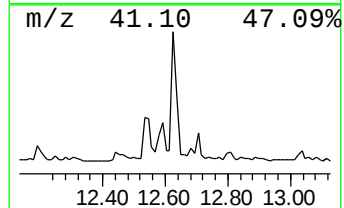
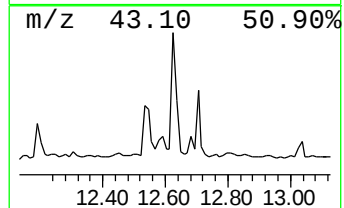
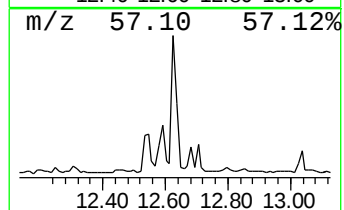
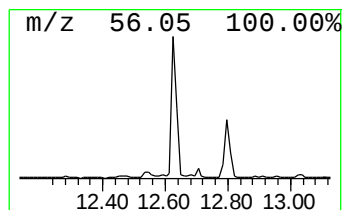
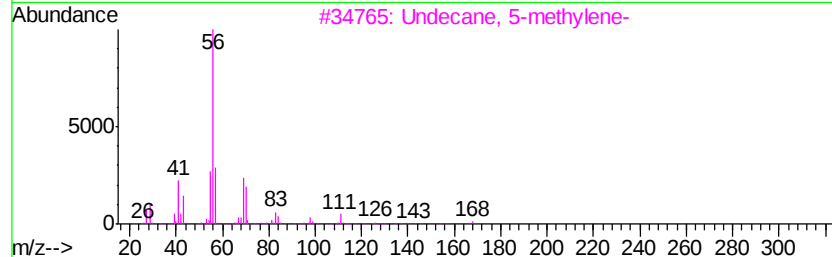
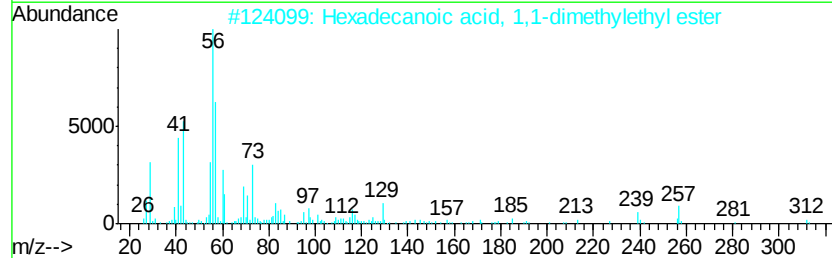
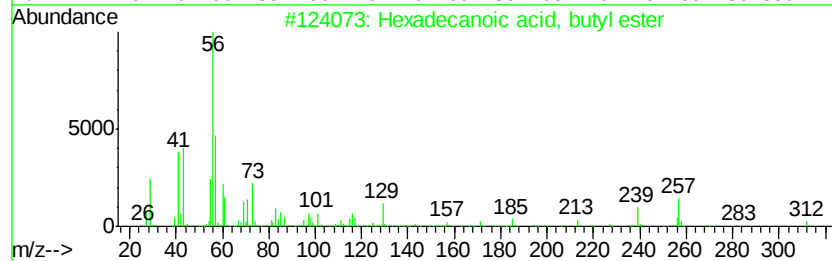
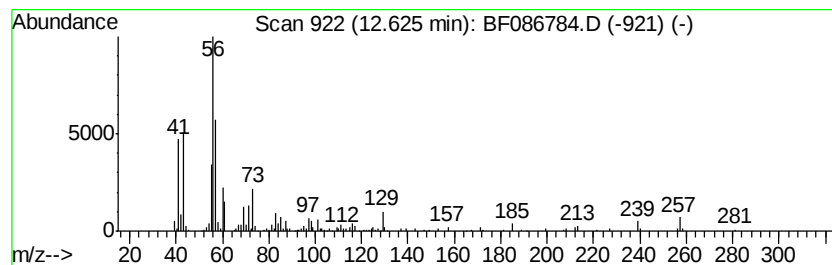
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	9.28 ng	252256	Chrysene-d12	13.85

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	49
3		Undecane, 5-methylene-	168	C12H24	005698-48-6	38
4		(S)-(-)-2-Azetidinecarboxylic acid	101	C4H7NO2	002133-34-8	38
5		Cyclobutanone, 3,3-dimethyl-	98	C6H10O	001192-33-2	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
Data File : BF086784.D
Acq On : 7 May 2016 20:04
Operator : UM/SJ
Sample : H2878-05
Misc :
ALS Vial : 54 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
URSMW-14

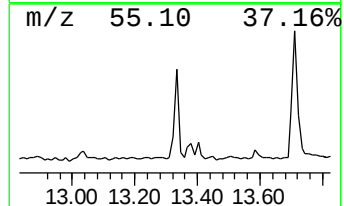
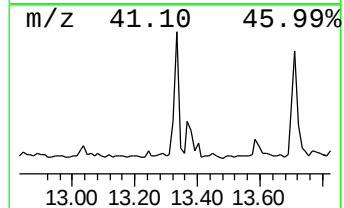
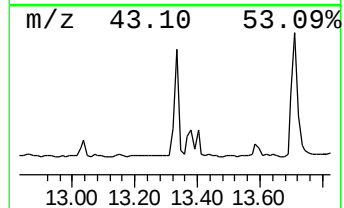
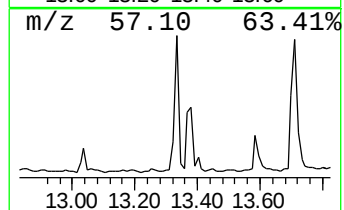
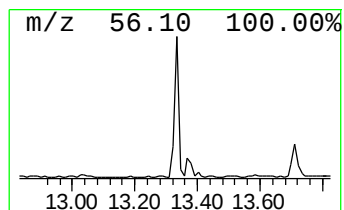
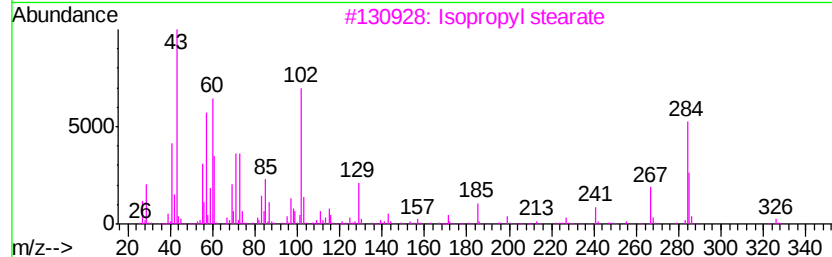
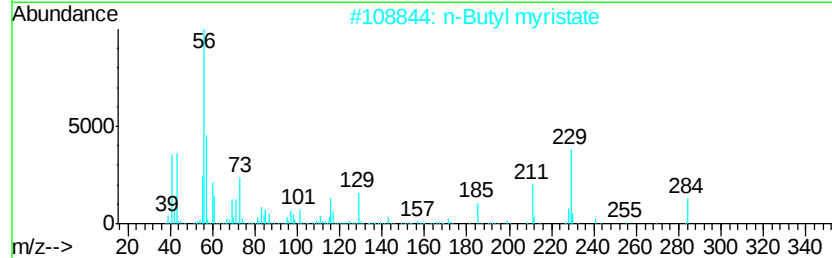
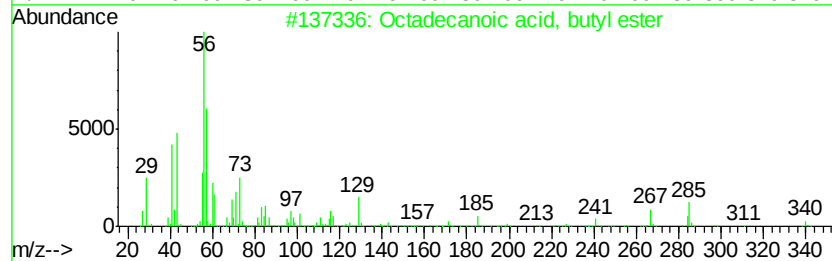
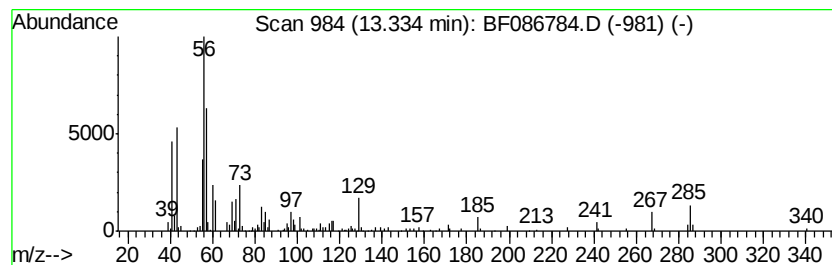
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.33	6.86 ng	186446	Chrysene-d12	13.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2		n-Butyl myristate	284	C18H36O2	000110-36-1	80
3		Isopropyl stearate	326	C21H42O2	000112-10-7	45
4		Octadecanoic acid	284	C18H36O2	000057-11-4	38
5		Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
Data File : BF086784.D
Acq On : 7 May 2016 20:04
Operator : UM/SJ
Sample : H2878-05
Misc :
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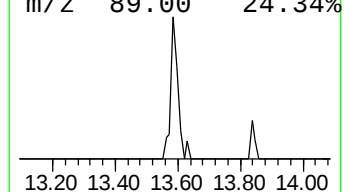
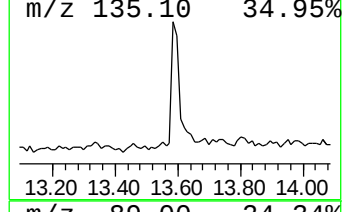
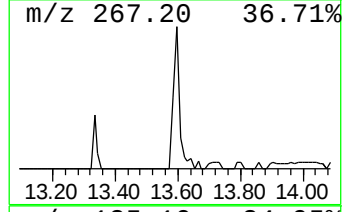
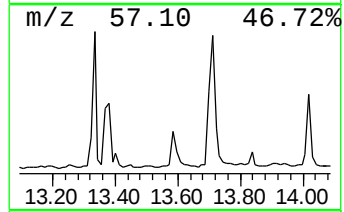
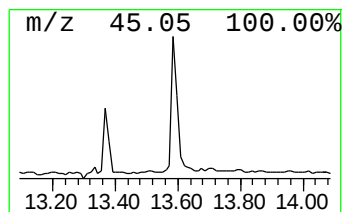
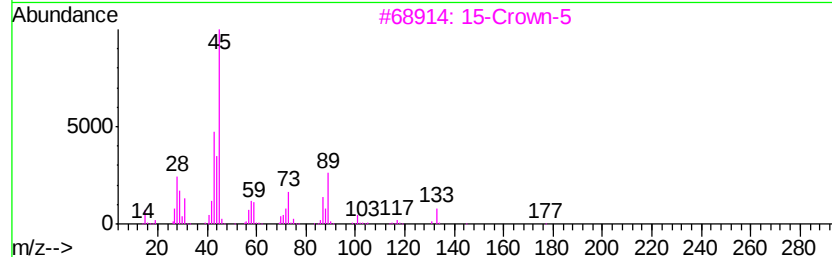
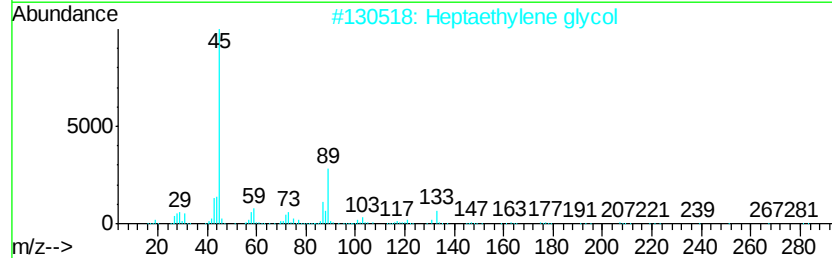
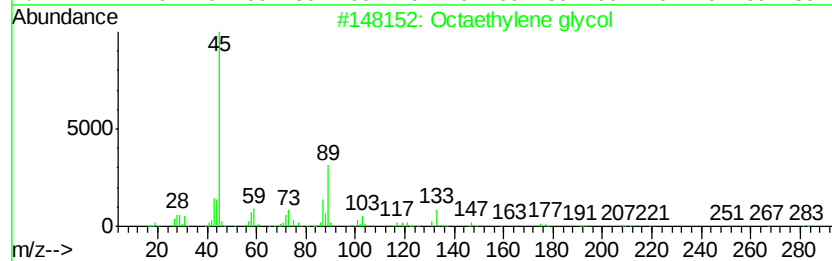
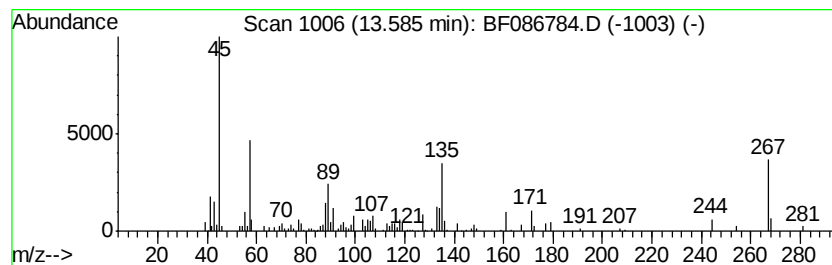
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octaethylene glycol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.59	4.39 ng	119240	Chrysene-d12		13.85	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octaethylene glycol	370	C16H34O9	1000289-34-2	37
2		Heptaethylene glycol	326	C14H30O8	005617-32-3	37
3		15-Crown-5	220	C10H20O5	033100-27-5	37
4		1,4,7,10,13,16-Hexaoxacyclooctad...	264	C12H24O6	017455-13-9	37
5		2-Butanone, 3-hydroxy-	88	C4H8O2	000513-86-0	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050716\
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Acq On : 7 May 2016 20:04
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Sample : H2878-05
Misc :
ALS Vial : 54 Sample Multiplier: 1

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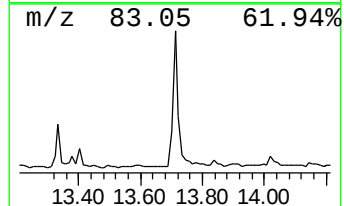
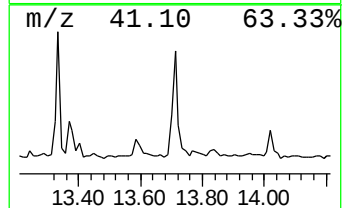
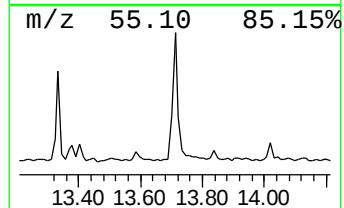
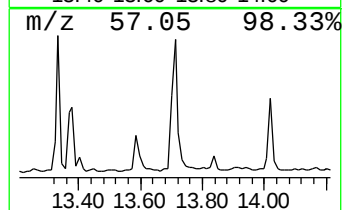
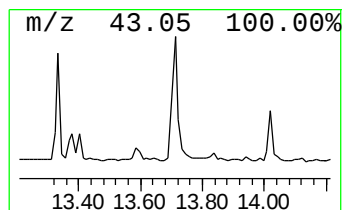
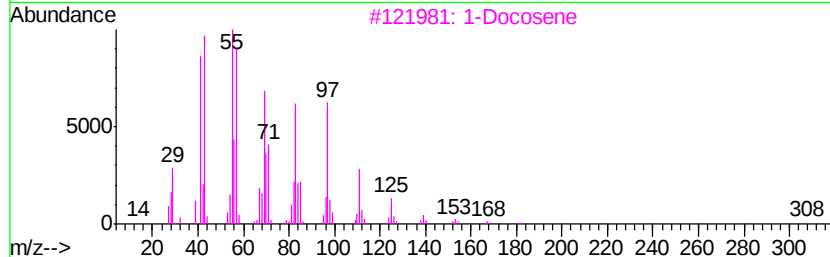
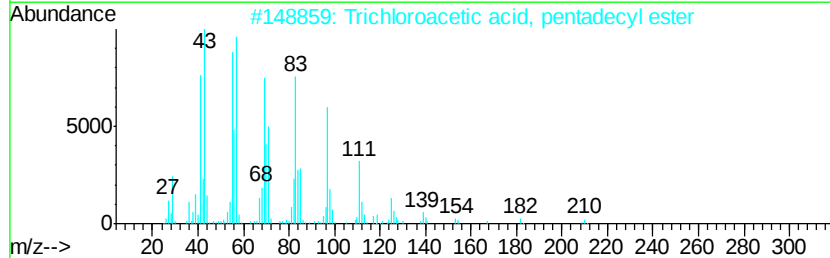
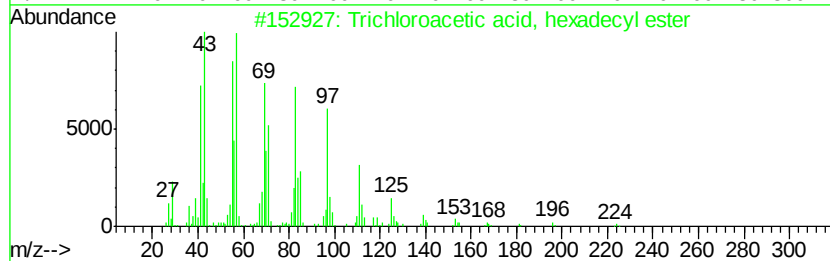
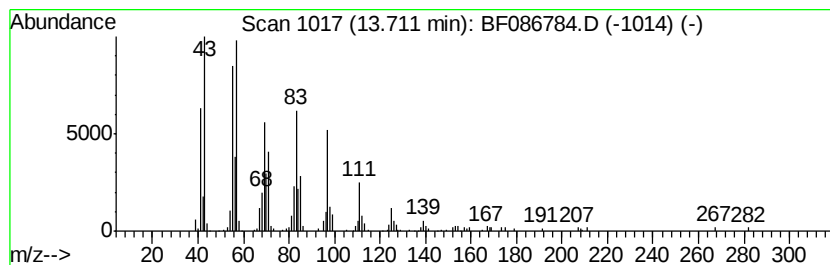
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	9.14 ng	248574	Chrysene-d12	13.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	95
3			1-Docosene	308	C22H44	001599-67-3	91
4			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
5			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91



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Acq On : 7 May 2016 20:04
Operator : UM/SJ
Sample : H2878-05
Misc :
ALS Vial : 54 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.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...	4.88	6.8 ng		206398	1	6.70	1205600	40.0
unknown6.48	6.48	178.0 ng		5363990	1	6.70	1205600	40.0
Eicosane	10.65	4.2 ng		156776	4	11.22	1494050	40.0
n-Hexadecanoic acid	11.76	5.8 ng		215298	4	11.22	1494050	40.0
Pentadecanoic acid	12.55	5.2 ng		141126	5	13.85	1087440	40.0
Ethanol, 2-[2-[4-...	12.59	6.0 ng		161656	5	13.85	1087440	40.0
Hexadecanoic acid...	12.63	9.3 ng		252256	5	13.85	1087440	40.0
Octadecanoic acid...	13.33	6.9 ng		186446	5	13.85	1087440	40.0
Octaethylene glycol	13.59	4.4 ng		119240	5	13.85	1087440	40.0
Trichloroacetic a...	13.71	9.1 ng		248574	5	13.85	1087440	40.0