

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060816\
 Data File : BF087835.D
 Acq On : 9 Jun 2016 5:45
 Operator : UM/SJ
 Sample : H3405-06
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-01-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	1.667	4	7	10	rVB	3889120	5832408	100.00%	18.274%
2	1.747	13	14	24	rVV	430578	748786	12.84%	2.346%
3	1.884	24	26	40	rVB	1981377	3139751	53.83%	9.837%
4	2.067	40	42	68	rVB2	63474	362678	6.22%	1.136%
5	5.004	296	299	306	rVB	110428	159298	2.73%	0.499%
6	5.427	332	336	338	rVB	1975472	2474052	42.42%	7.752%
7	6.456	423	426	429	rBV	1742168	2228138	38.20%	6.981%
8	6.593	435	438	440	rBV	2455030	2275819	39.02%	7.130%
9	6.822	456	458	461	rBV	648279	602317	10.33%	1.887%
10	6.982	469	472	474	rBV	2178947	1853403	31.78%	5.807%
11	7.393	505	508	510	rBV	1528352	1640382	28.13%	5.140%
12	8.113	568	571	573	rBV	874252	810537	13.90%	2.540%
13	9.188	663	665	668	rBV	1948786	2568240	44.03%	8.047%
14	9.588	698	700	702	rBV	303447	243083	4.17%	0.762%
15	9.862	722	724	727	rVB	540678	757200	12.98%	2.372%
16	10.651	791	793	796	rBV2	1079878	1199111	20.56%	3.757%
17	11.348	852	854	857	rVB	739100	620339	10.64%	1.944%
18	12.765	976	978	981	rBV	77117	74944	1.28%	0.235%
19	12.937	991	993	996	rBV	1772285	1856995	31.84%	5.818%
20	13.428	1033	1036	1038	rBV	315881	502421	8.61%	1.574%
21	13.497	1041	1042	1047	rVB2	41893	66536	1.14%	0.208%
22	13.851	1071	1073	1079	rBV	64378	104809	1.80%	0.328%
23	13.988	1082	1085	1087	rVV	576331	631165	10.82%	1.978%
24	14.114	1093	1096	1100	rBV	37743	78407	1.34%	0.246%
25	14.754	1149	1152	1156	rBV	431328	608541	10.43%	1.907%
26	15.405	1206	1209	1212	rBV	405812	477387	8.19%	1.496%

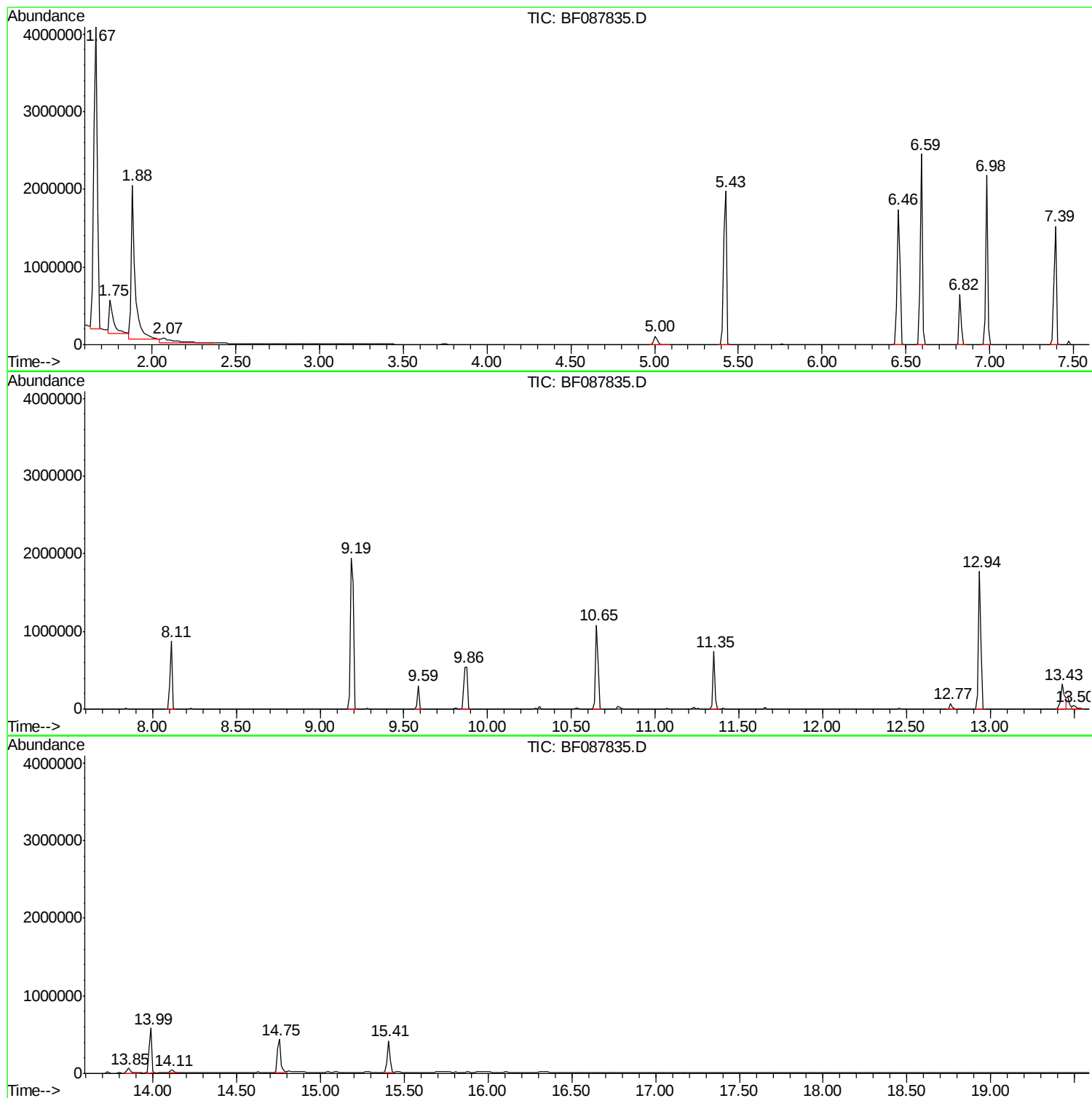
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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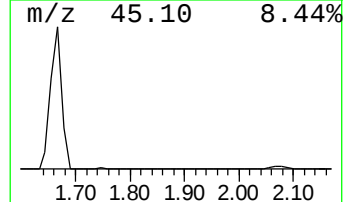
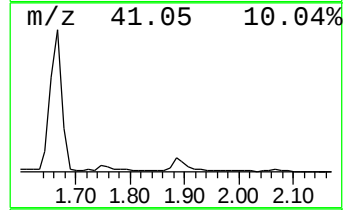
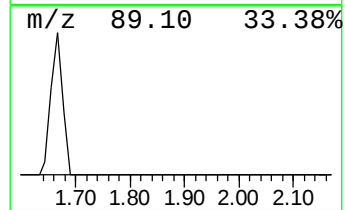
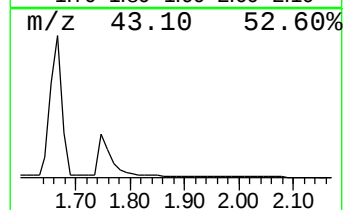
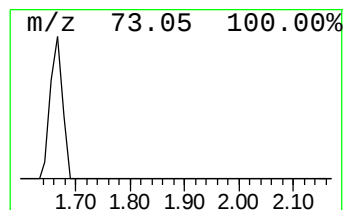
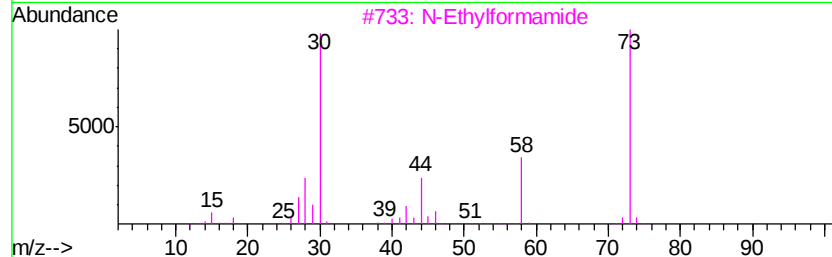
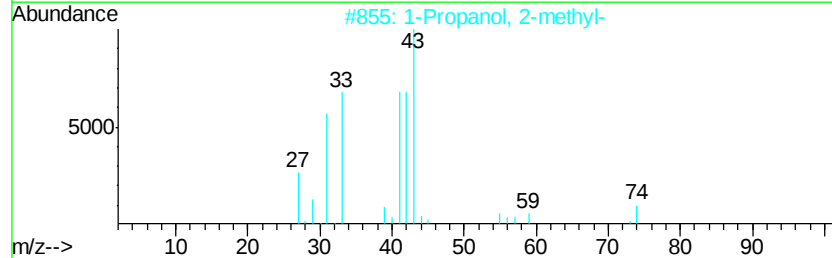
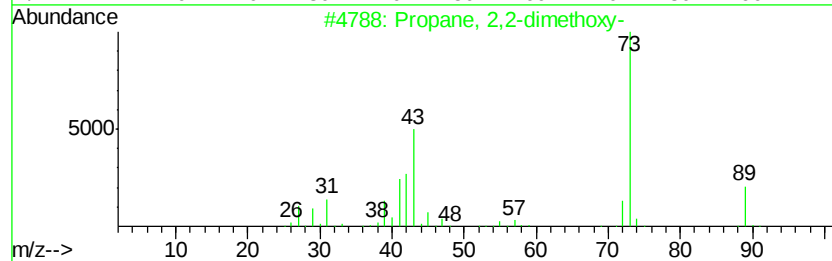
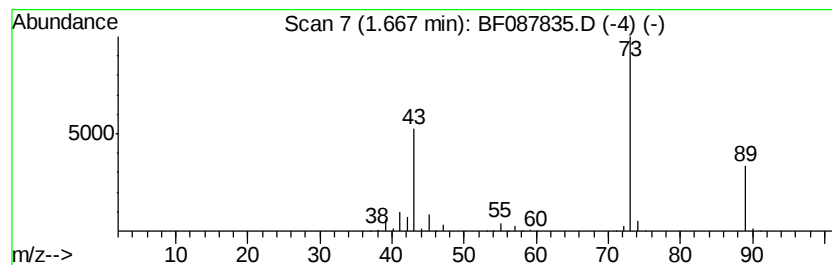
Instrument :
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ClientSampleId :
SB-01-COMP-0.5-11.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.67	193.67 ng	5832410	1,4-Dichlorobenzene-d4	6.82	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	1,3-Diaminoquanidine	89	CH7N5	004364-78-7	9
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9



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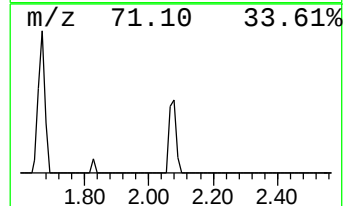
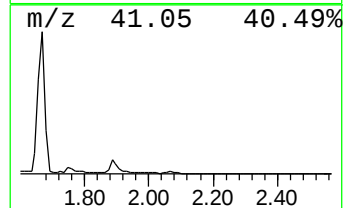
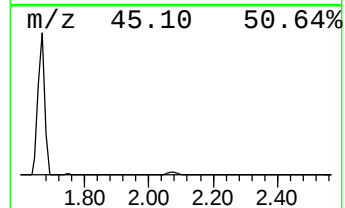
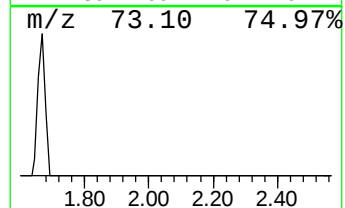
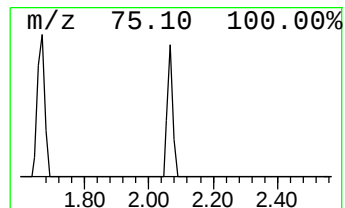
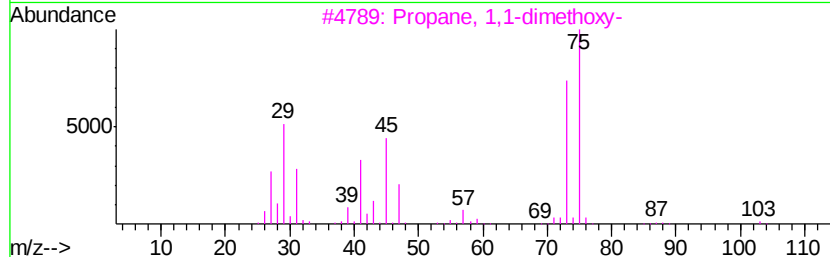
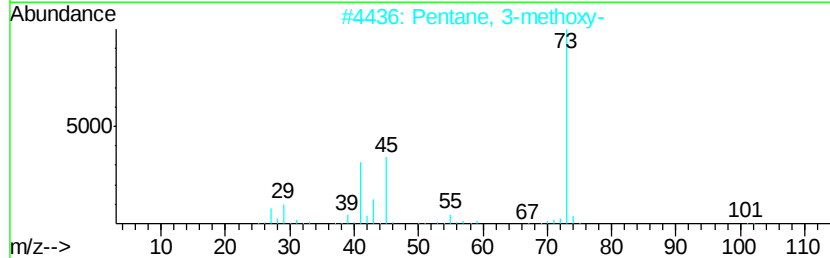
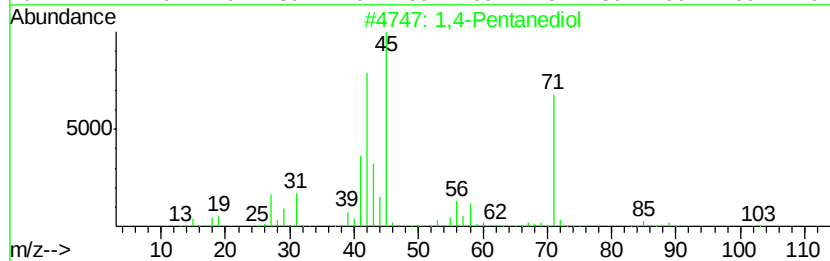
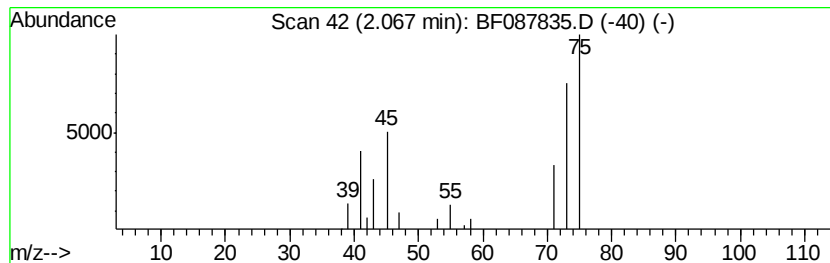
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Peak Number 4 unknown2.07 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.07	12.04 ng	362678	1,4-Dichlorobenzene-d4	6.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Pentanediol	104	C5H12O2	000626-95-9	4
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	4
3			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	4
4			1-Butanamine, N-nitro-	118	C4H10N2O2	003182-75-0	4
5			Isoamyl lactate	160	C8H16O3	019329-89-6	4



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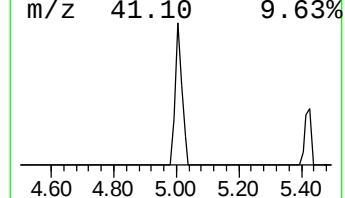
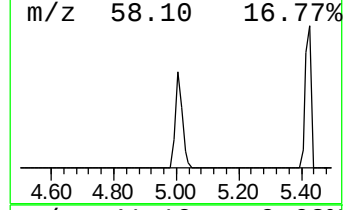
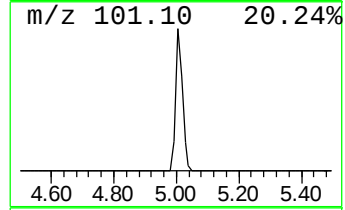
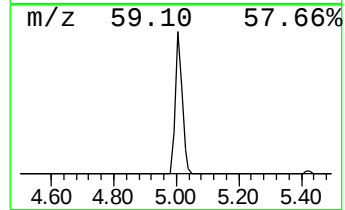
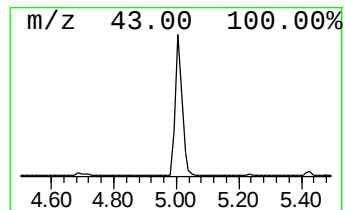
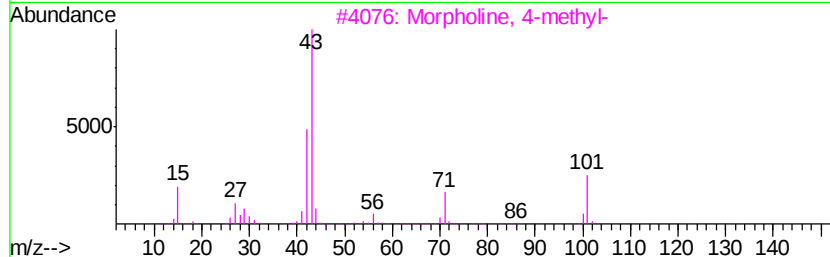
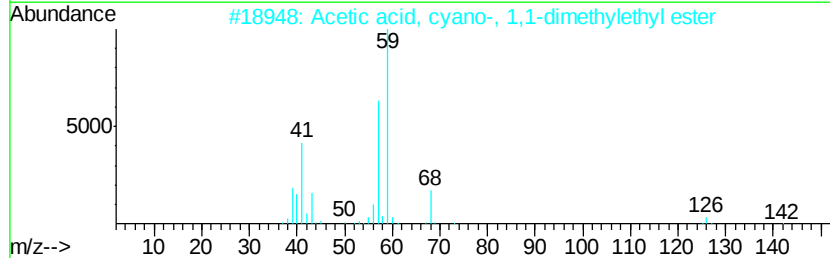
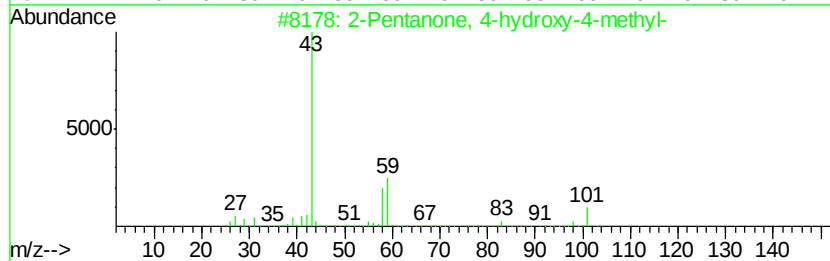
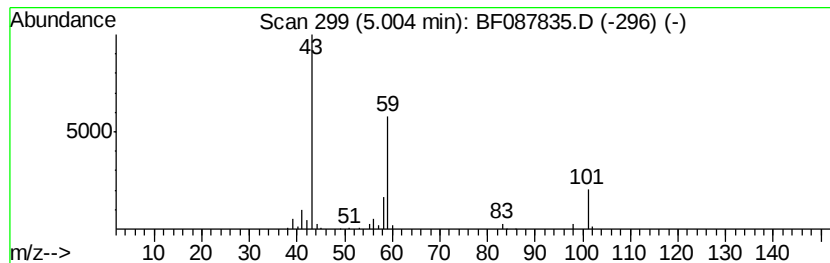
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Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	5.29 ng	159298	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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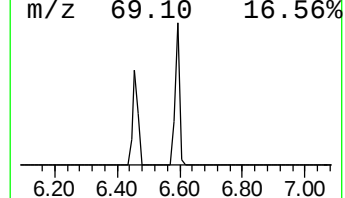
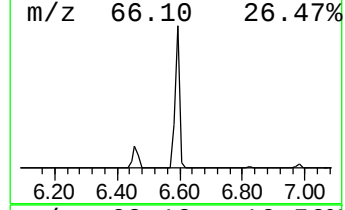
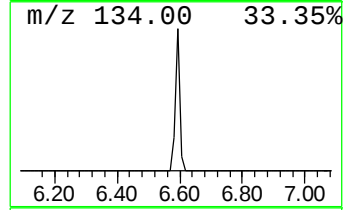
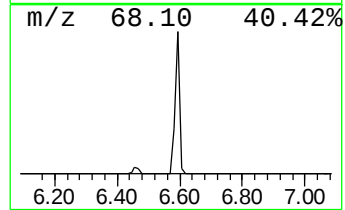
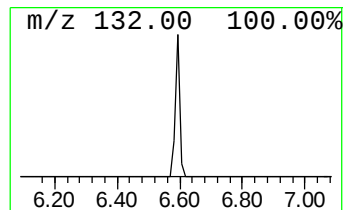
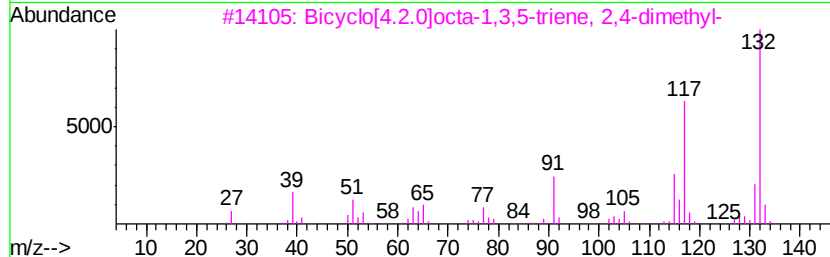
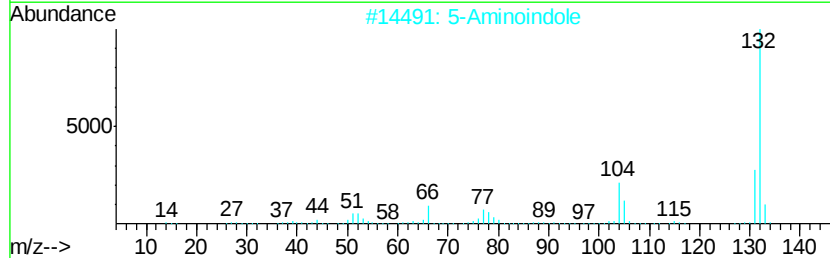
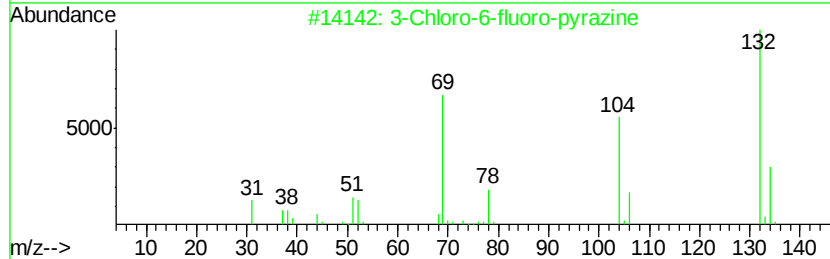
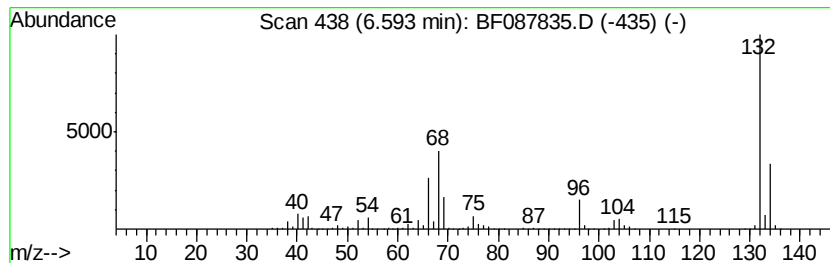
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Peak Number 6 unknown6.59 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	75.57 ng	2275820	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			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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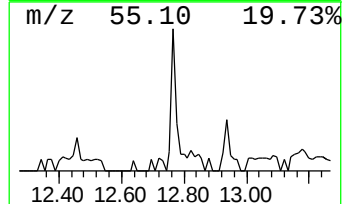
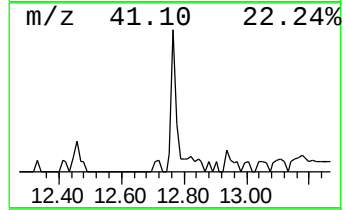
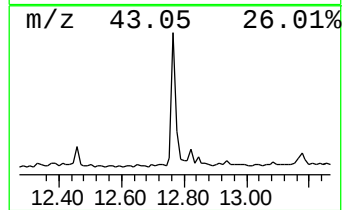
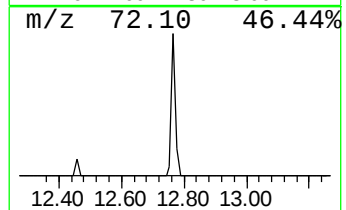
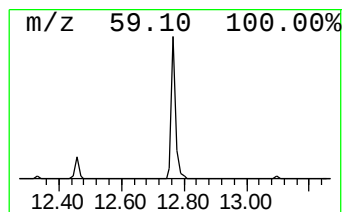
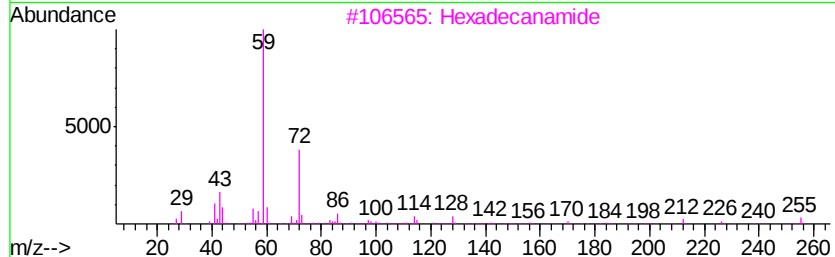
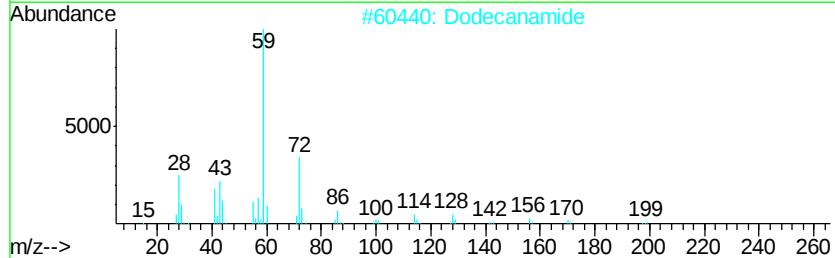
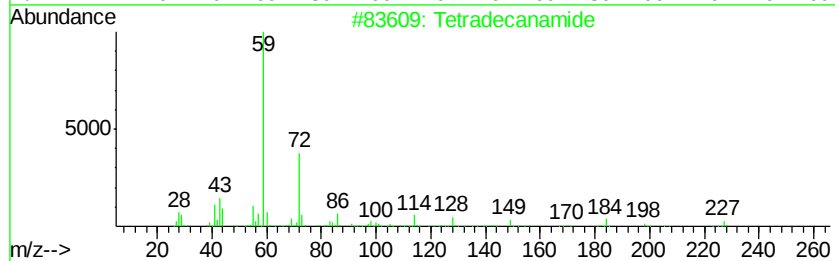
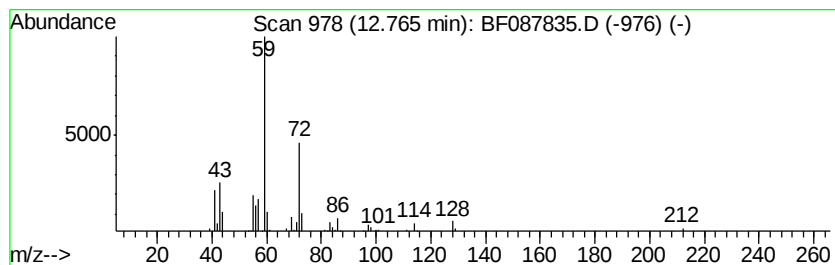
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Peak Number 8 Tetradecanamide Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	2.37 ng	74944	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetradecanamide	227	C14H29NO	000638-58-4	90
2		Dodecanamide	199	C12H25NO	001120-16-7	86
3		Hexadecanamide	255	C16H33NO	000629-54-9	83
4		Decanamide-	171	C10H21NO	002319-29-1	83
5		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	74



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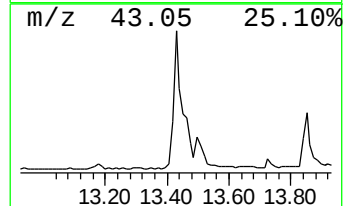
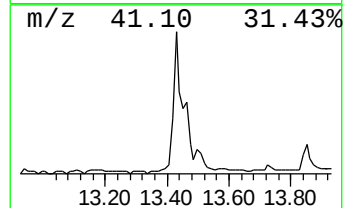
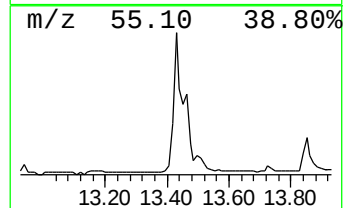
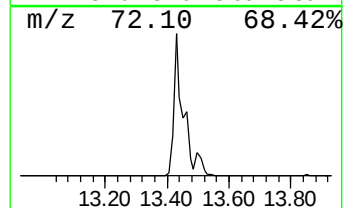
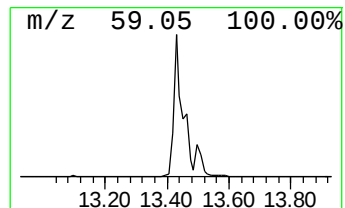
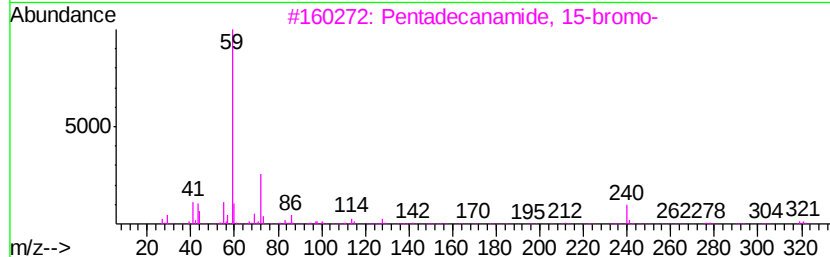
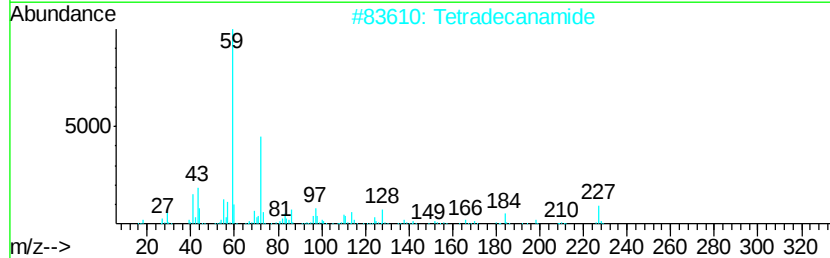
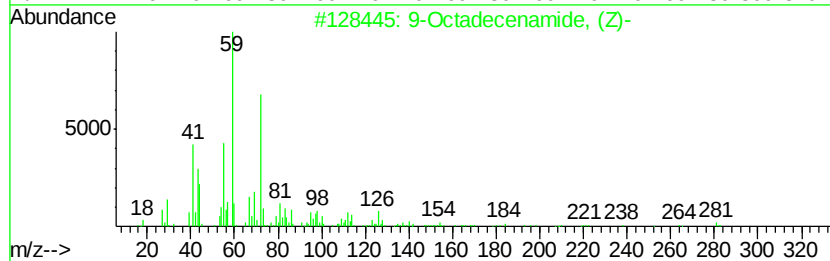
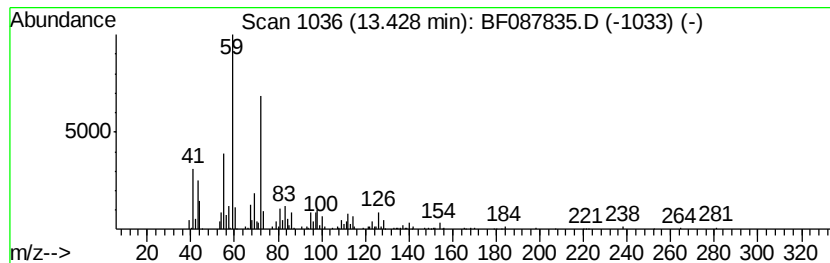
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.43	15.92 ng	502421	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2		Tetradecanamide	227	C14H29NO	000638-58-4	72
3		Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	64
4		Dodecanamide	199	C12H25NO	001120-16-7	59
5		Octanamide	143	C8H17NO	000629-01-6	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060816\
Data File : BF087835.D
Acq On : 9 Jun 2016 5:45
Operator : UM/SJ
Sample : H3405-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-01-COMP-0.5-11.0

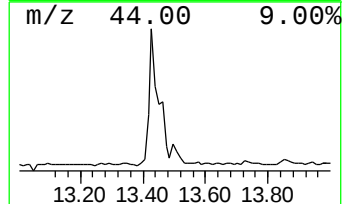
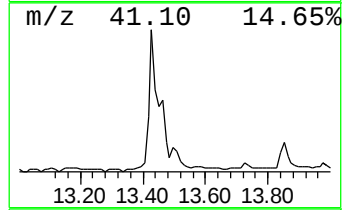
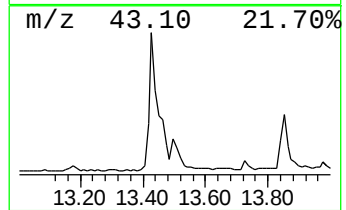
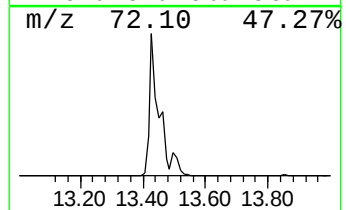
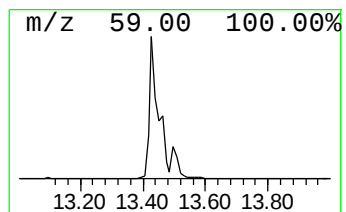
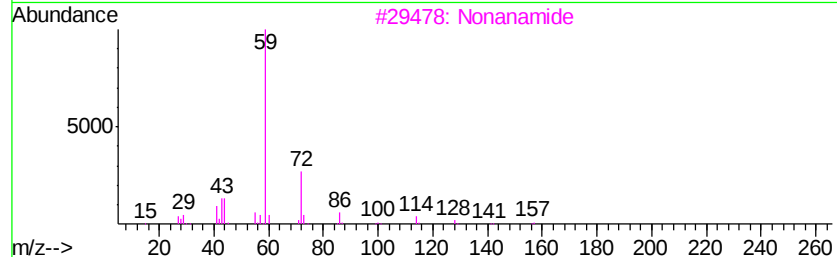
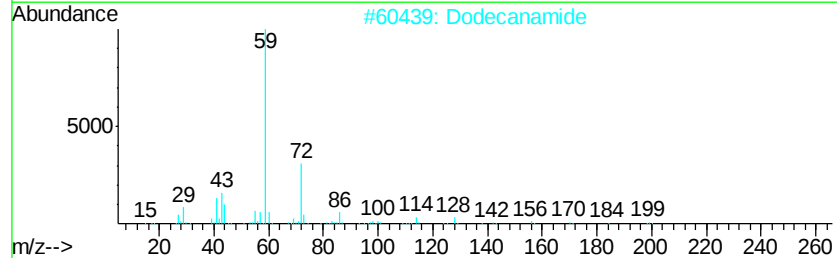
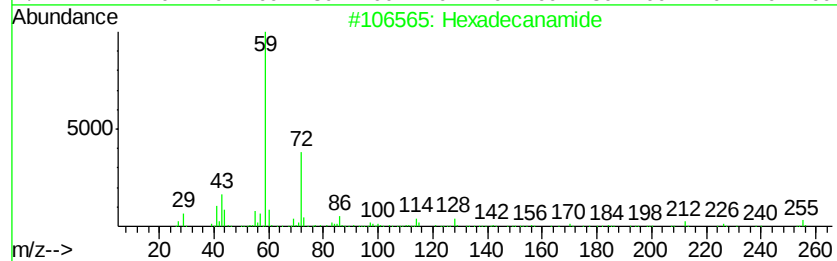
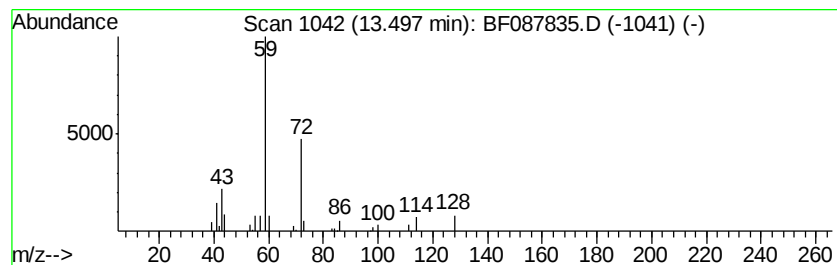
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexadecanamide Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	2.11 ng	66536	Chrysene-d12	13.99

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanamide	255	C16H33NO	000629-54-9	83
2			Dodecanamide	199	C12H25NO	001120-16-7	72
3			Nonanamide	157	C9H19NO	001120-07-6	50
4			2-Pentanol, 2,3-dimethyl-	116	C7H16O	004911-70-0	37
5			Hexanamide, 4-ethyl-5,5-dimethyl-	171	C10H21NO	054789-39-8	28



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060816\
Data File : BF087835.D
Acq On : 9 Jun 2016 5:45
Operator : UM/SJ
Sample : H3405-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

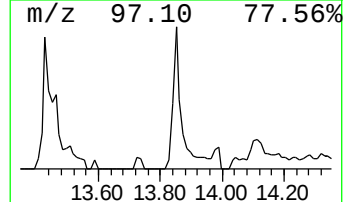
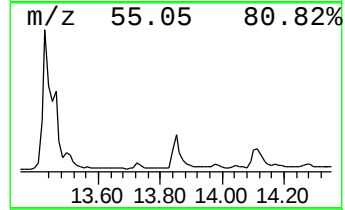
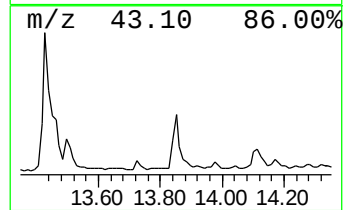
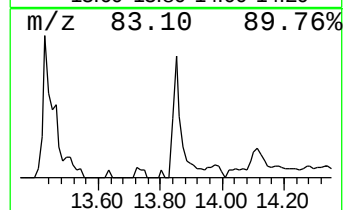
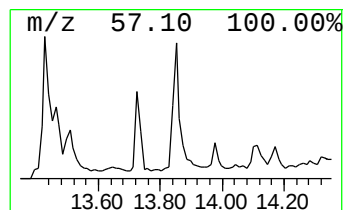
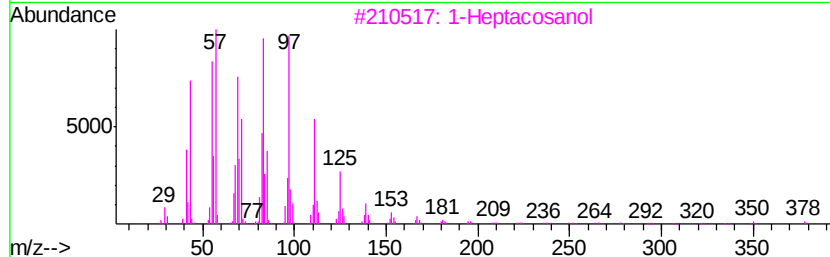
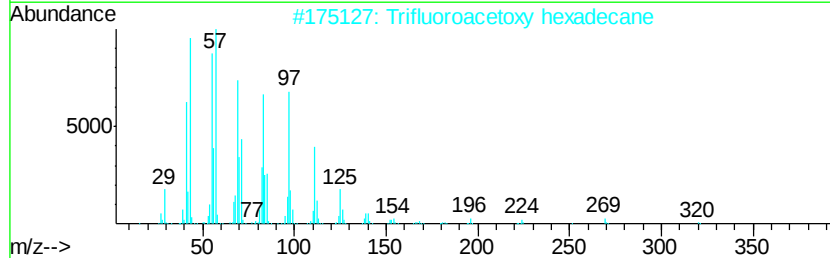
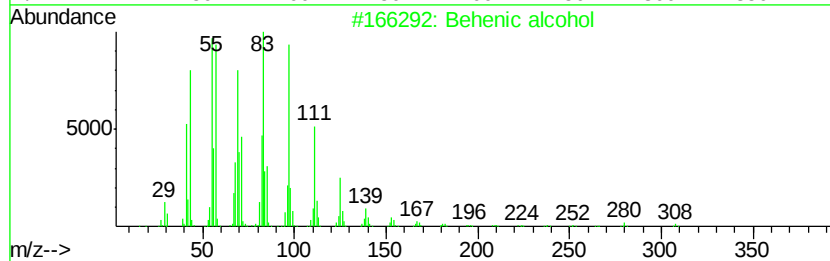
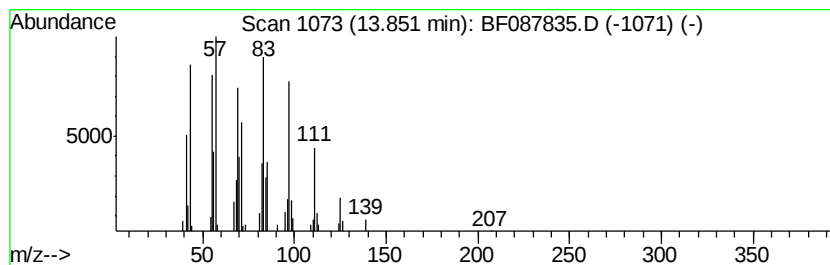
Instrument :
BNA_F
ClientSampleId :
SB-01-COMP-0.5-11.0

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

Peak Number 11 Behenic alcohol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.		
13.85	3.32 ng	104809	Chrysene-d12		13.99		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	94
2			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3			1-Heptacosanol	396	C27H56O	002004-39-9	93
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060816\
Data File : BF087835.D
Acq On : 9 Jun 2016 5:45
Operator : UM/SJ
Sample : H3405-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-01-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
Propane, 2,2-dime...	1.67	193.7	ng	5832410	1	6.82	602317	20.0
unknown2.07	2.07	12.0	ng	362678	1	6.82	602317	20.0
2-Pentanone, 4-hy...	5.00	5.3	ng	159298	1	6.82	602317	20.0
unknown6.59	6.59	75.6	ng	2275820	1	6.82	602317	20.0
Tetradecanamide	12.77	2.4	ng	74944	5	13.99	631165	20.0
9-Octadecenamide, ...	13.43	15.9	ng	502421	5	13.99	631165	20.0
Hexadecanamide	13.50	2.1	ng	66536	5	13.99	631165	20.0
Behenic alcohol	13.85	3.3	ng	104809	5	13.99	631165	20.0