

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011116\
 Data File : BF084378.D
 Acq On : 11 Jan 2016 14:30
 Operator : SJ/UM
 Sample : H1043-16
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-3COMP

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-BF123115.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	5.047	257	259	268	rVB	1427466	2319544	26.86%	3.176%
2	5.470	293	296	299	rBV	6026957	8110581	93.92%	11.105%
3	6.510	383	387	389	rBV	7099248	8489436	98.31%	11.624%
4	6.636	395	398	400	rBV	6697938	8635395	100.00%	11.823%
5	6.853	415	417	419	rBV	2020071	1626675	18.84%	2.227%
6	6.922	421	423	425	rBV	129320	111797	1.29%	0.153%
7	7.013	428	431	433	rVB	6688084	5999472	69.48%	8.214%
8	7.424	464	467	469	rBV	4961033	5235760	60.63%	7.169%
9	8.145	527	530	532	rBV	1982914	2090793	24.21%	2.863%
10	9.219	621	624	627	rBV	7417286	7259556	84.07%	9.940%
11	9.493	646	648	650	rBV	349395	280138	3.24%	0.384%
12	9.619	656	659	660	rBV	987629	1315170	15.23%	1.801%
13	9.825	675	677	681	rBV	153673	218174	2.53%	0.299%
14	9.893	681	683	686	rVB	2480590	2170343	25.13%	2.972%
15	10.328	719	721	723	rVB	439166	361312	4.18%	0.495%
16	10.545	737	740	744	rBV	114930	226533	2.62%	0.310%
17	10.682	749	752	755	rVV2	3920246	5065264	58.66%	6.935%
18	10.796	759	762	769	rVB2	621246	952785	11.03%	1.305%
19	10.991	777	779	784	rBV2	49843	105486	1.22%	0.144%
20	11.253	800	802	803	rBV	199127	201004	2.33%	0.275%
21	11.379	811	813	815	rBV	2314497	1962919	22.73%	2.688%
22	11.436	815	818	822	rVB2	39168	86988	1.01%	0.119%
23	12.796	934	937	939	rBV	299380	408029	4.73%	0.559%
24	12.865	939	943	947	rVV2	168647	332917	3.86%	0.456%
25	12.968	949	952	955	rBV	6096939	5778044	66.91%	7.911%
26	13.494	996	998	1000	rBV	317438	293264	3.40%	0.402%
27	13.871	1029	1031	1037	rBV	205641	300422	3.48%	0.411%
28	14.019	1041	1044	1046	rBV	999138	1366349	15.82%	1.871%
29	14.339	1070	1072	1074	rBV	124852	131601	1.52%	0.180%
30	14.488	1083	1085	1089	rBV	78274	96567	1.12%	0.132%
31	14.785	1107	1111	1114	rBV2	58093	117102	1.36%	0.160%
32	14.865	1116	1118	1121	rVB	187119	194391	2.25%	0.266%
33	15.448	1166	1169	1171	rBV	763063	1192759	13.81%	1.633%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

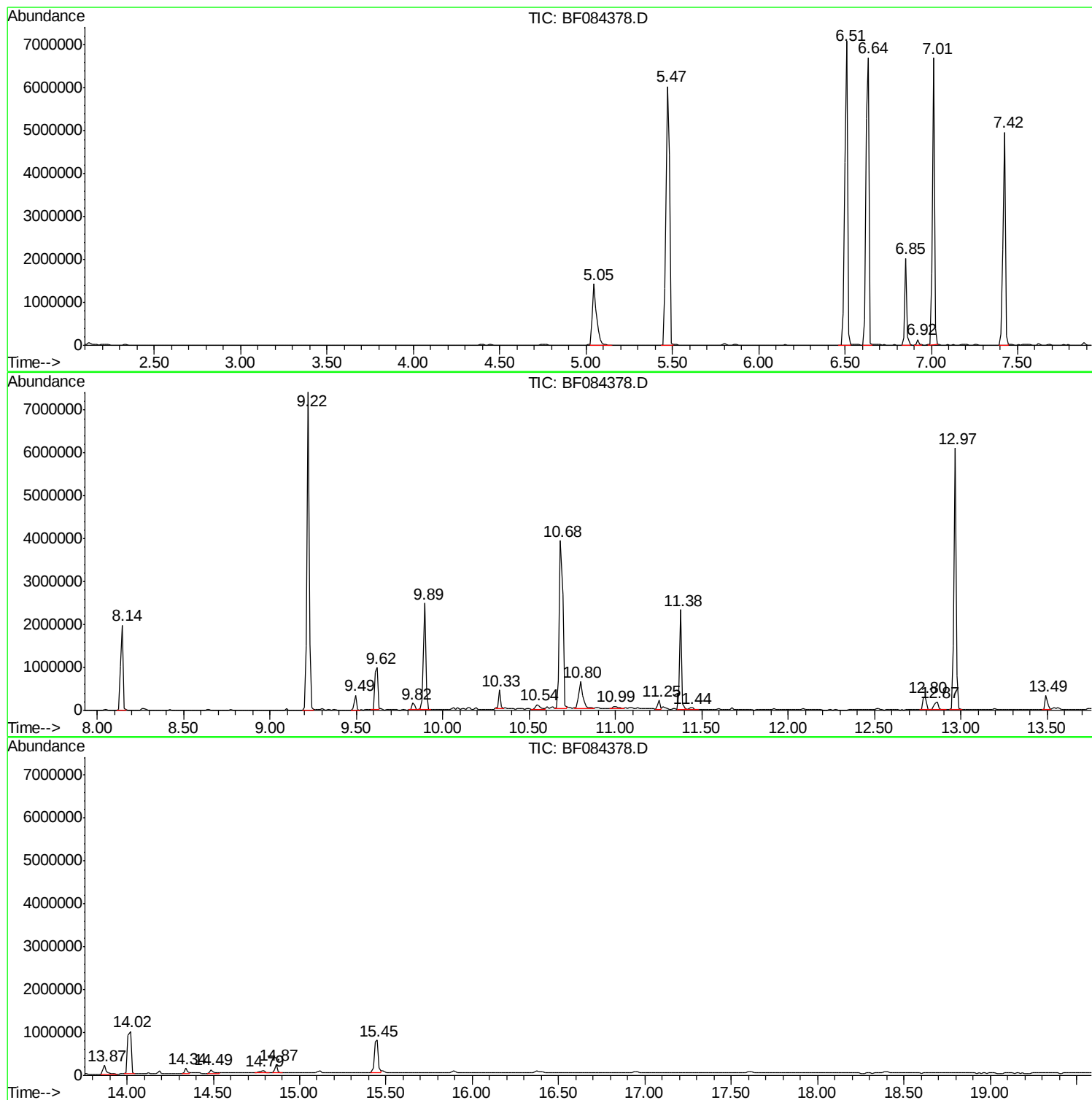
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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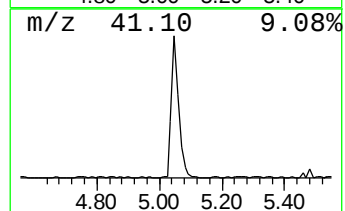
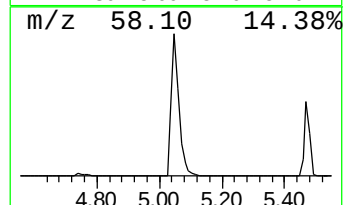
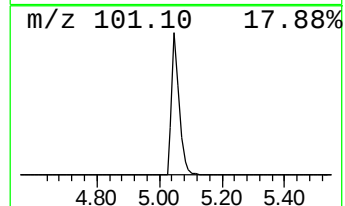
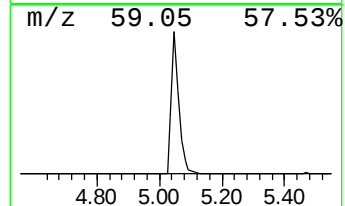
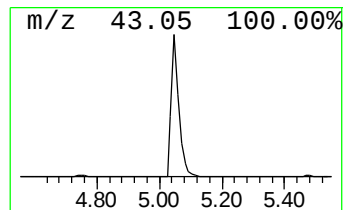
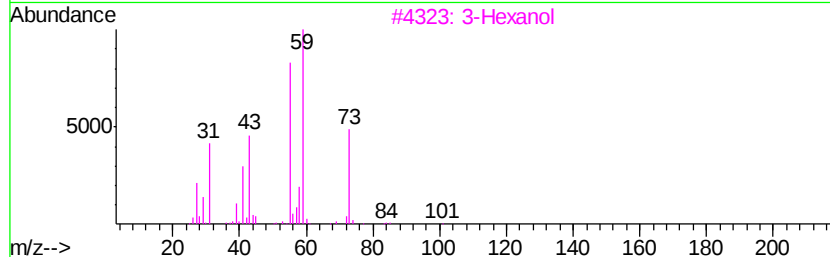
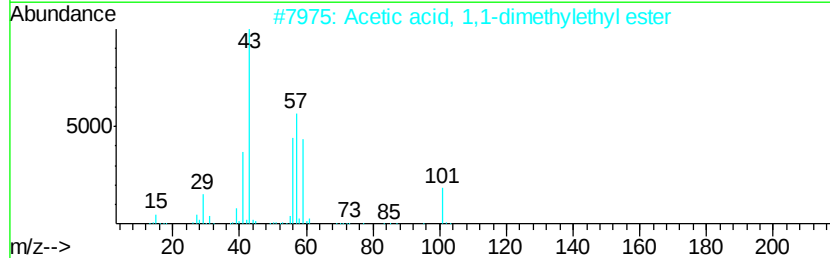
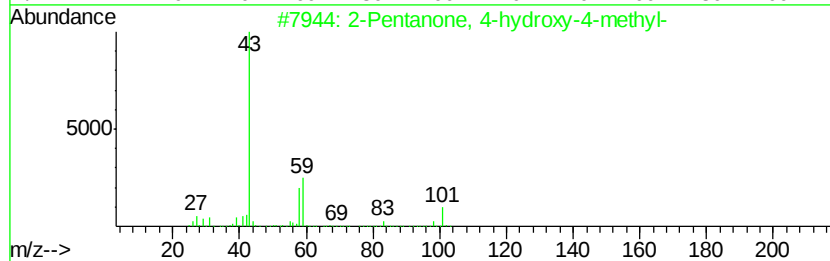
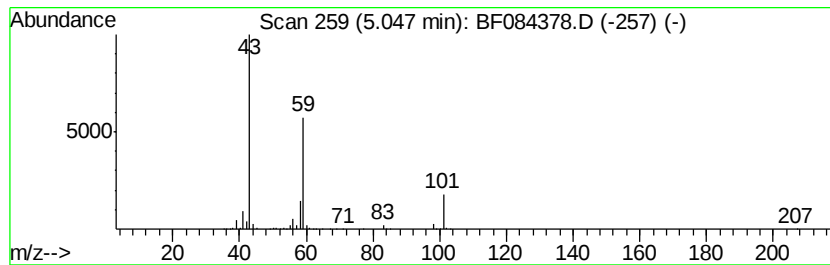
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	28.52 ng	2319540	1,4-Dichlorobenzene-d4	6.85

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	3-Hexanol	102	C6H14O	000623-37-0	33		
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33		



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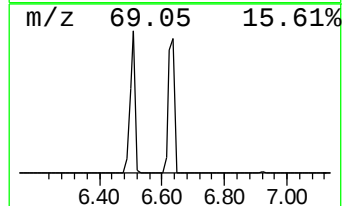
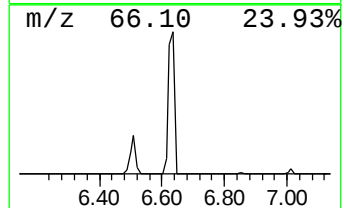
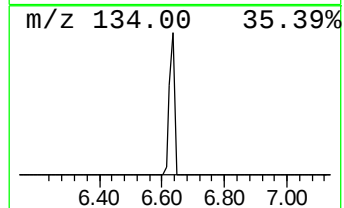
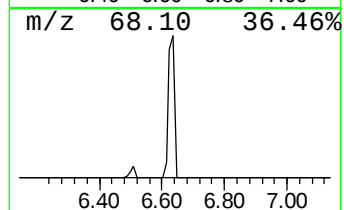
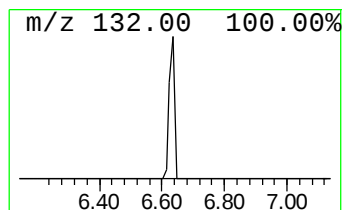
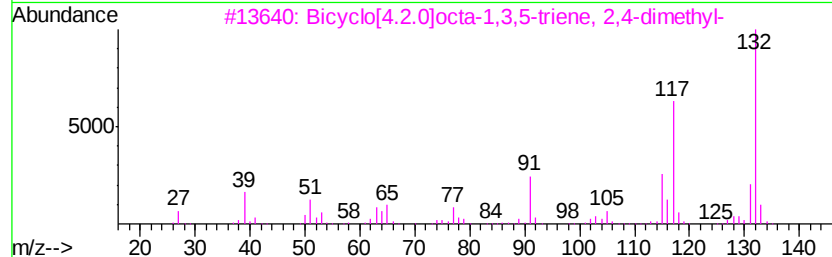
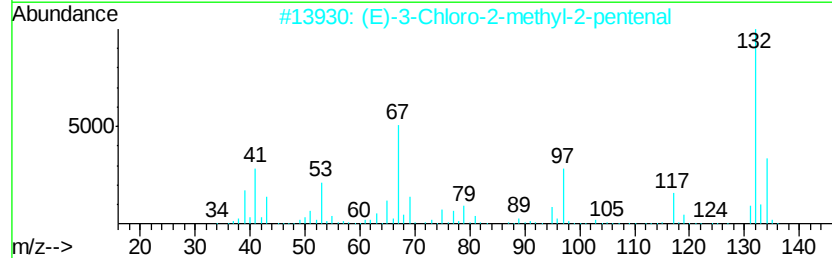
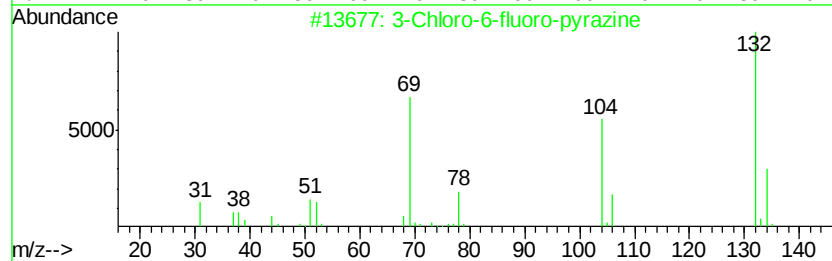
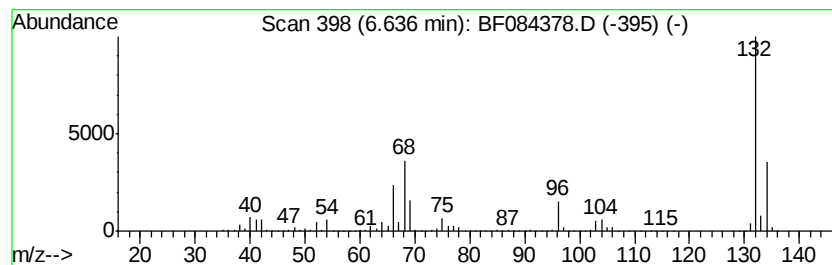
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Peak Number 2 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	106.17 ng	8635400	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
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		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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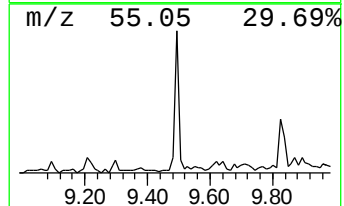
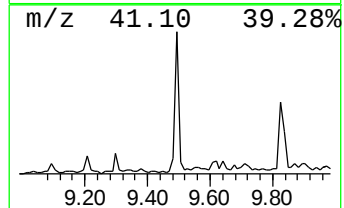
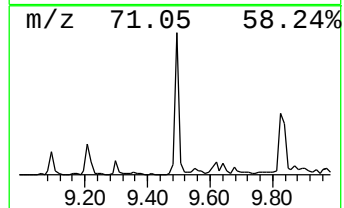
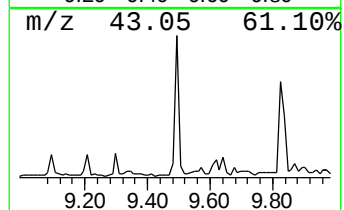
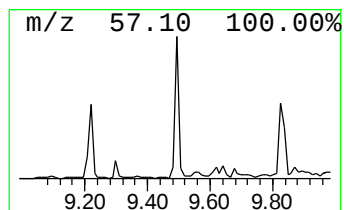
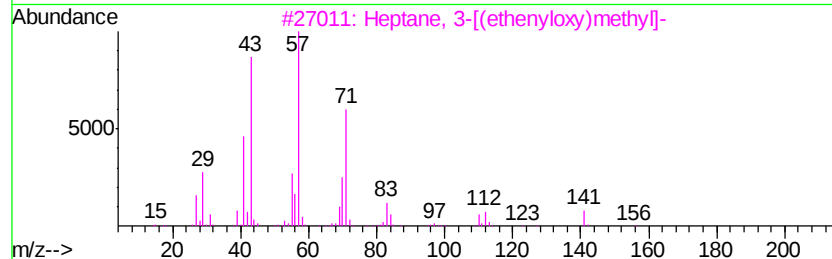
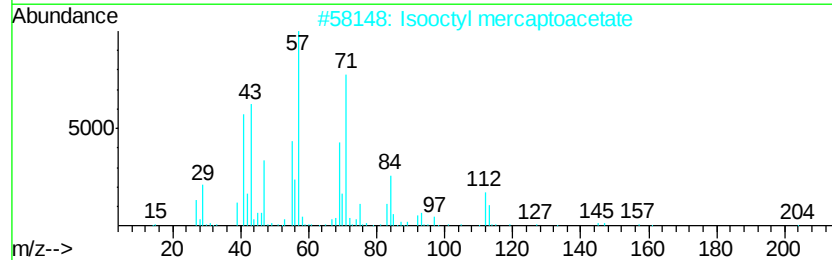
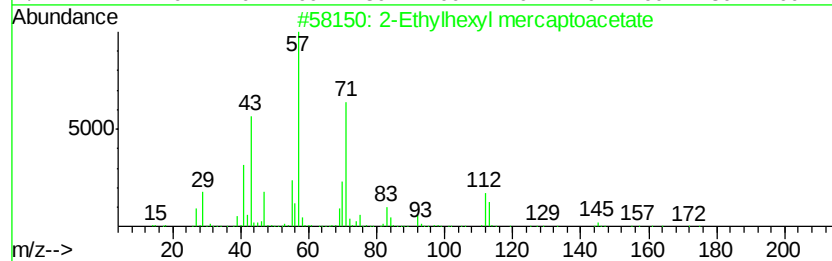
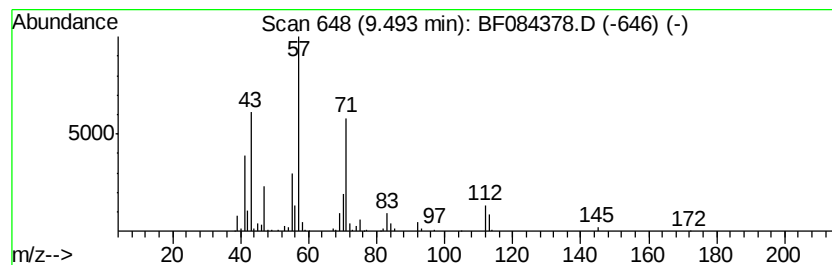
Instrument :
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Ethylhexyl mercaptoacetate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
9.49	2.58 ng	280138	Acenaphthene-d10		9.89
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethylhexyl mercaptoacetate	204	C10H20O2S	007659-86-1	86
2	Isooctyl mercaptoacetate	204	C10H20O2S	025103-09-7	72
3	Heptane, 3-[(ethenyloxy)methyl]-	156	C10H20O	000103-44-6	53
4	Decane, 4-methyl-	156	C11H24	002847-72-5	50
5	Undecane, 6-ethyl-	184	C13H28	017312-60-6	50



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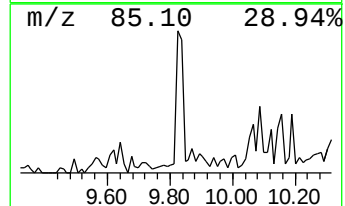
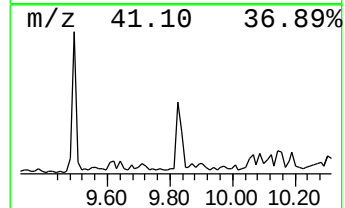
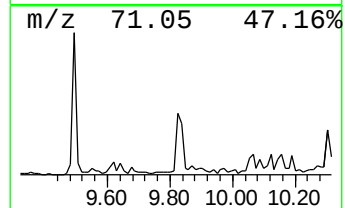
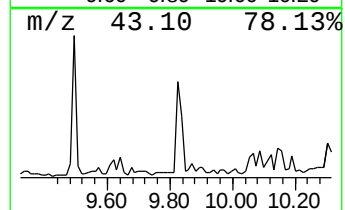
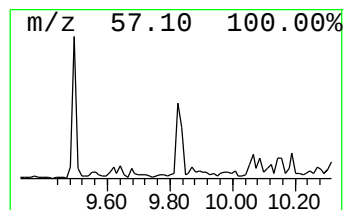
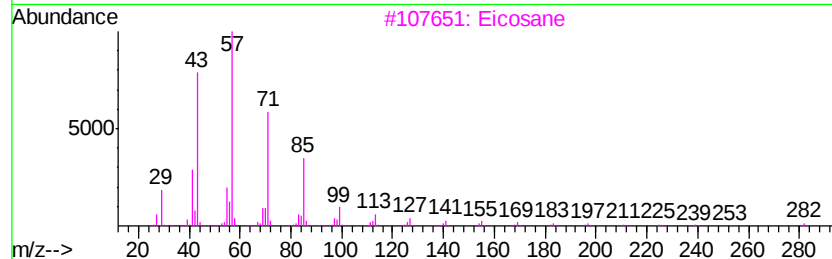
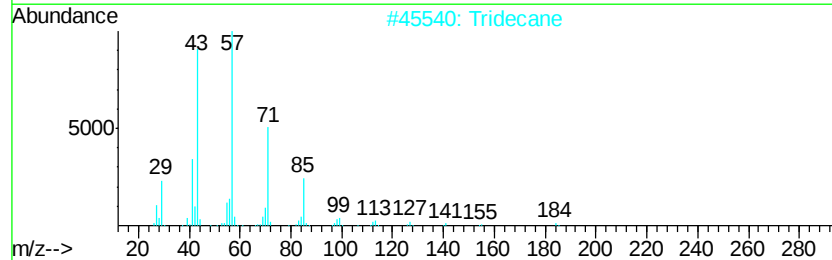
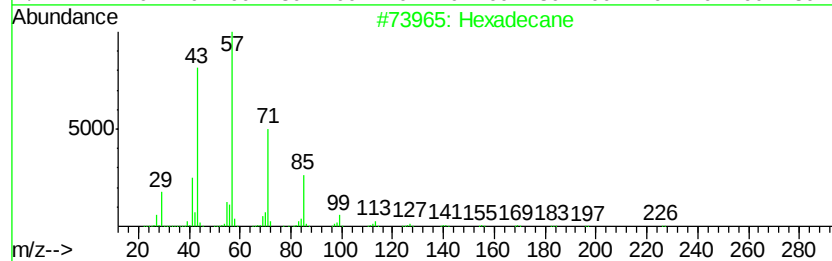
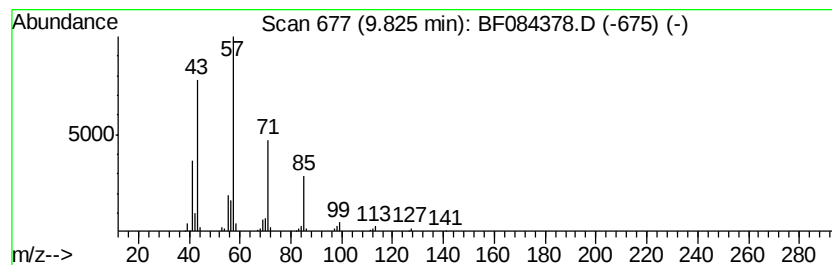
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.82	2.01 ng	218174	Acenaphthene-d10	9.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	91
2		Tridecane	184	C13H28	000629-50-5	83
3		Eicosane	282	C20H42	000112-95-8	72
4		Decane, 2,9-dimethyl-	170	C12H26	001002-17-1	72
5		Undecane, 4,5-dimethyl-	184	C13H28	017312-79-7	72



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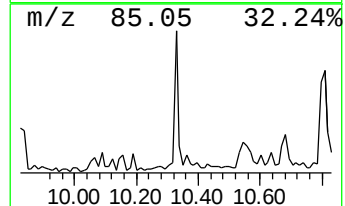
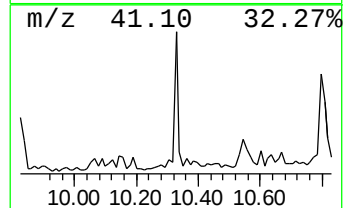
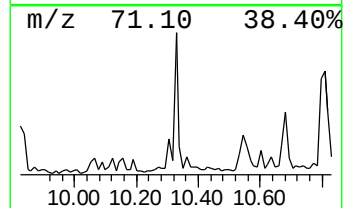
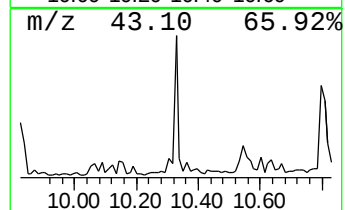
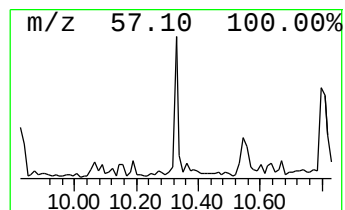
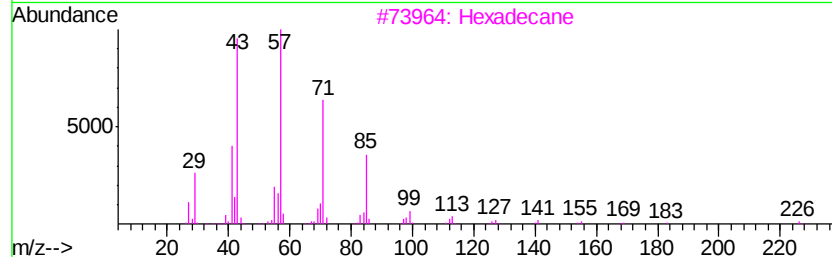
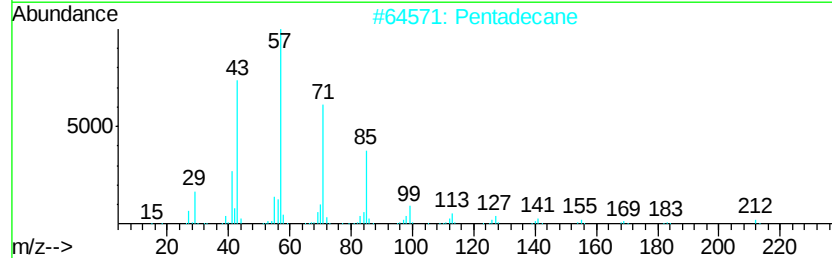
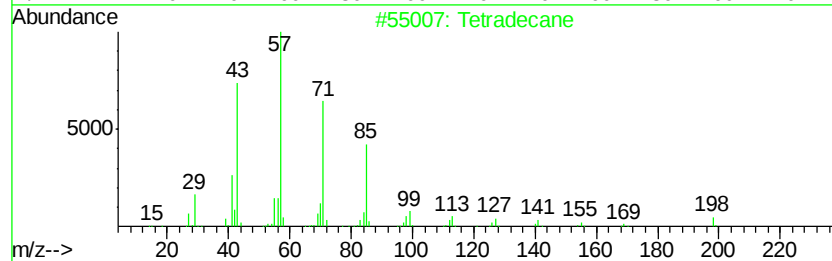
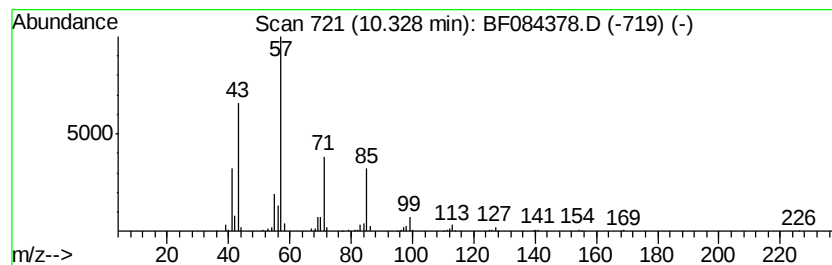
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Tetradecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.33	3.33 ng	361312	Acenaphthene-d10	9.89
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Tetradecane	198 C14H30	000629-59-4 90
2		Pentadecane	212 C15H32	000629-62-9 83
3		Hexadecane	226 C16H34	000544-76-3 80
4		Eicosane	282 C20H42	000112-95-8 64
5		Octane, 2,4,6-trimethyl-	156 C11H24	062016-37-9 59



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SB-3COMP

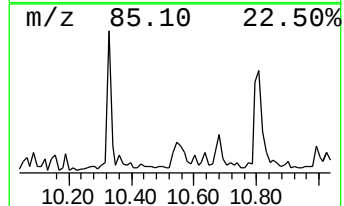
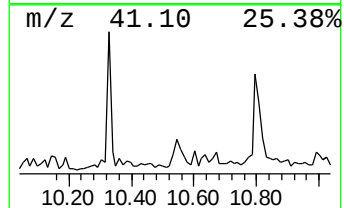
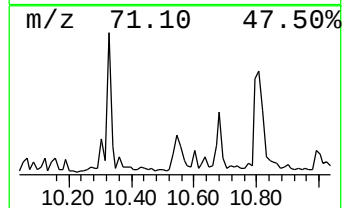
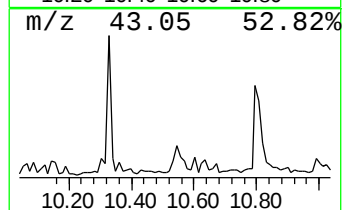
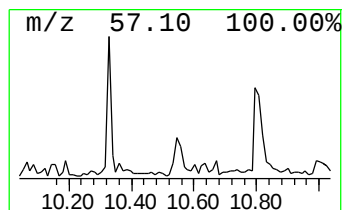
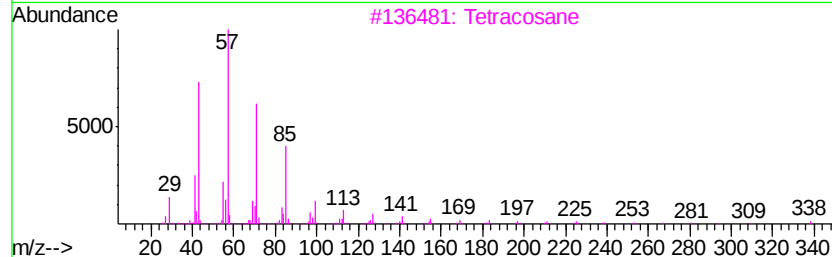
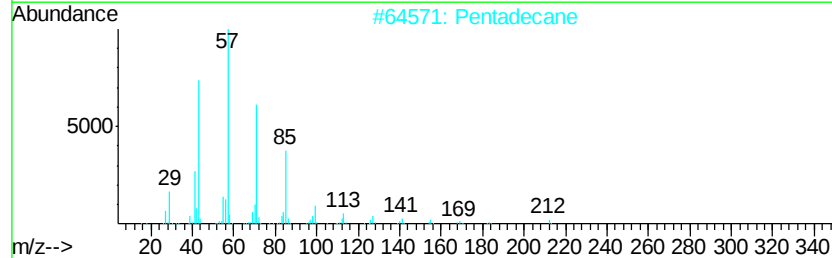
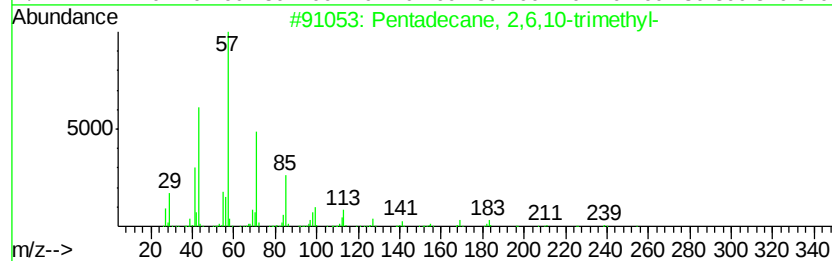
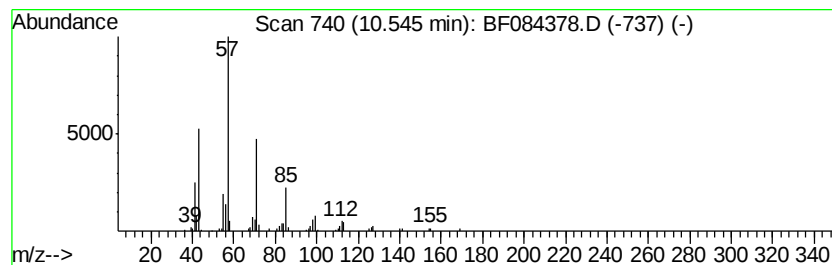
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentadecane, 2,6,10-trimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.54	2.09 ng	226533	Acenaphthene-d10	9.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	90
2		Pentadecane	212	C15H32	000629-62-9	80
3		Tetracosane	338	C24H50	000646-31-1	80
4		Eicosane	282	C20H42	000112-95-8	74
5		Tridecane, 6-methyl-	198	C14H30	013287-21-3	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011116\
Data File : BF084378.D
Acq On : 11 Jan 2016 14:30
Operator : SJ/UM
Sample : H1043-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

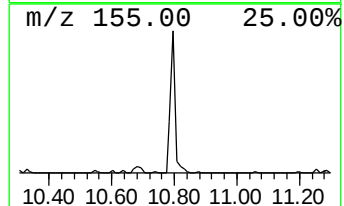
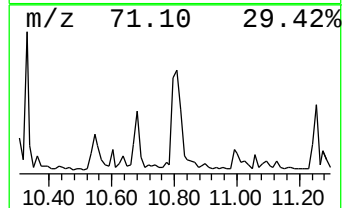
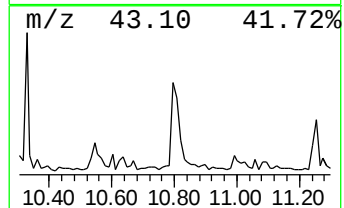
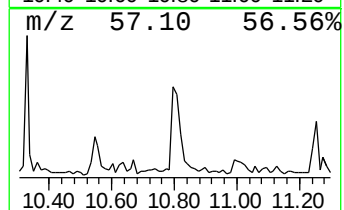
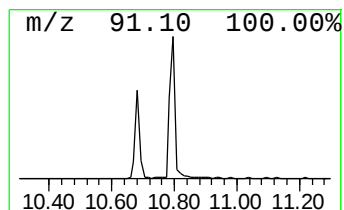
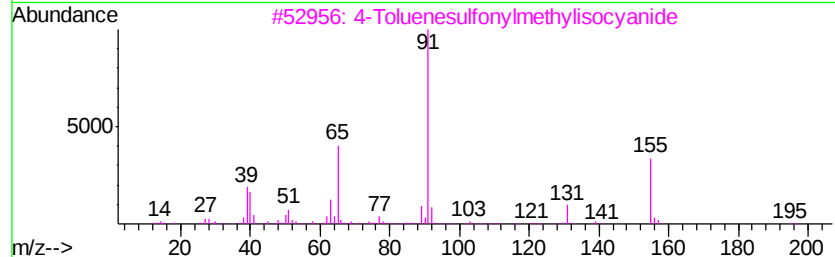
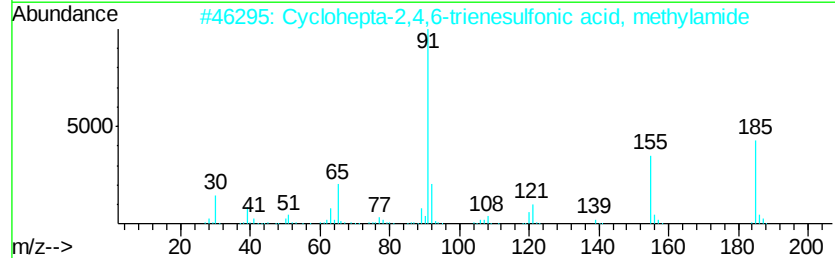
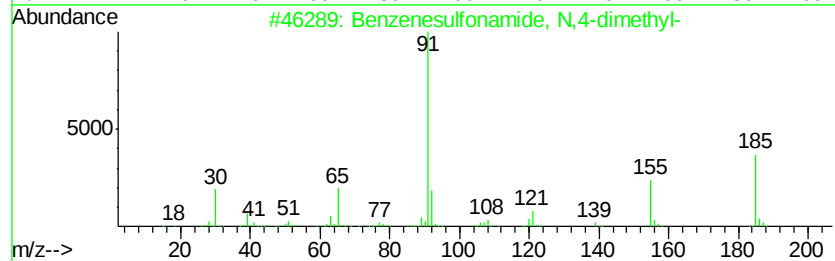
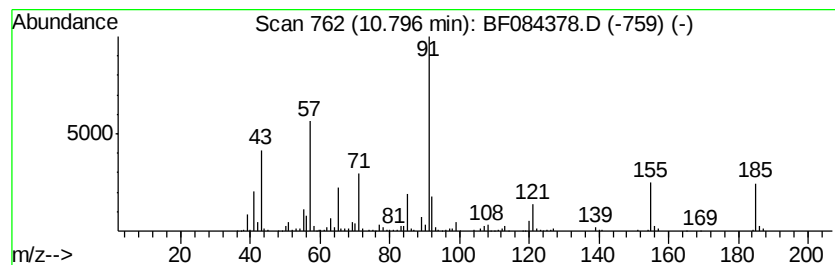
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzenesulfonamide, N,4-dim... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.80	9.71 ng	952785	Phenanthrene-d10	11.38	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	93
2	Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	53
3	4-Toluenesulfonylmethylisocyanide	195	C9H9NO2S	036635-61-7	38
4	(O-p-Tosylisonitroso)malononitrile	249	C10H7N3O3S	020893-01-0	38
5	1-Hydroxytricyclo[4.3.0.0(4,9)]n...	308	C16H20O4S	201992-83-8	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011116\
Data File : BF084378.D
Acq On : 11 Jan 2016 14:30
Operator : SJ/UM
Sample : H1043-16
Misc :
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Instrument :
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ClientSampleId :
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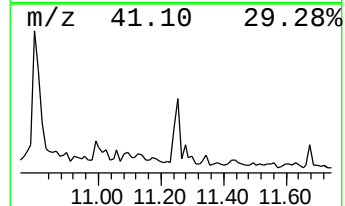
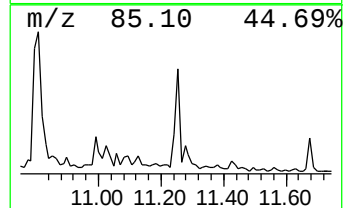
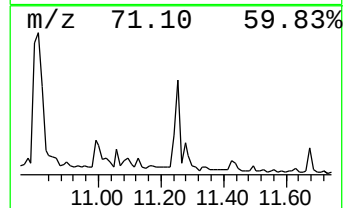
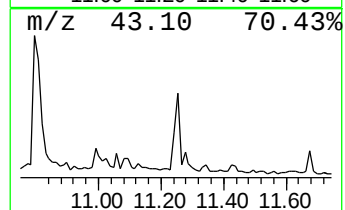
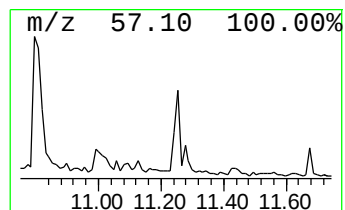
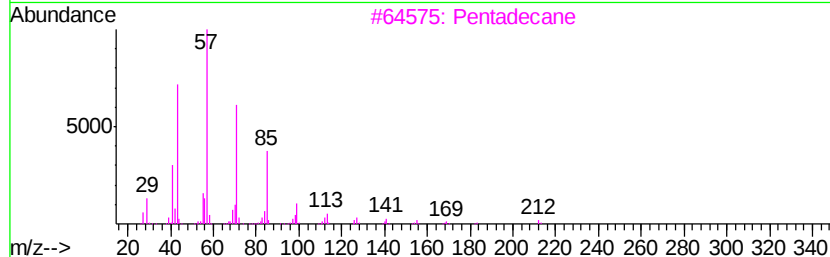
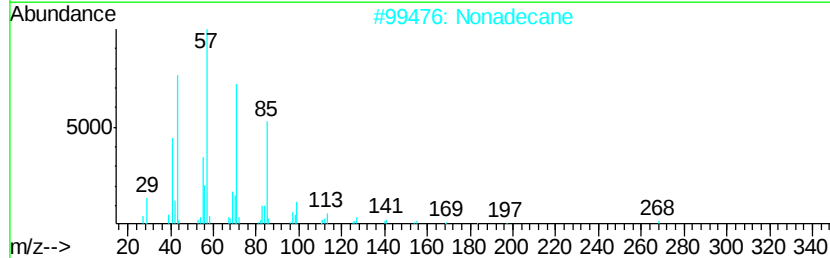
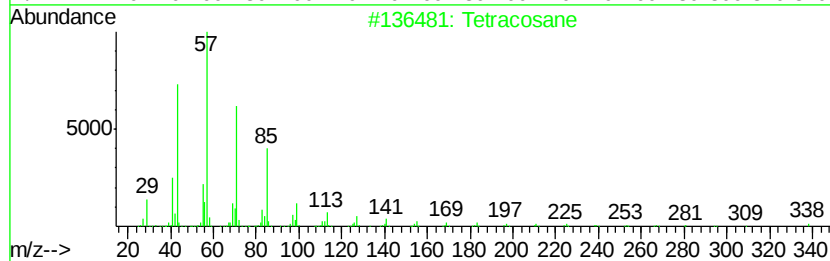
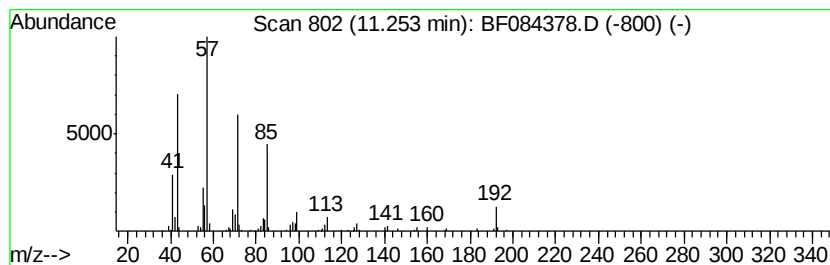
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetracosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.25	2.05 ng	201004	Phenanthrene-d10	11.38

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	87
2			Nonadecane	268	C19H40	000629-92-5	87
3			Pentadecane	212	C15H32	000629-62-9	87
4			Hexadecane	226	C16H34	000544-76-3	87
5			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011116\
Data File : BF084378.D
Acq On : 11 Jan 2016 14:30
Operator : SJ/UM
Sample : H1043-16
Misc :
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Instrument :
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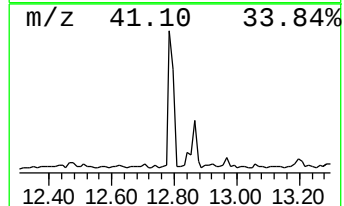
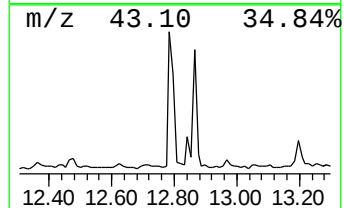
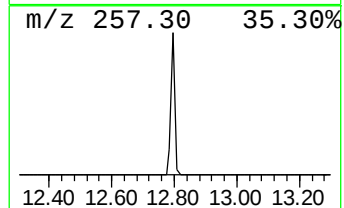
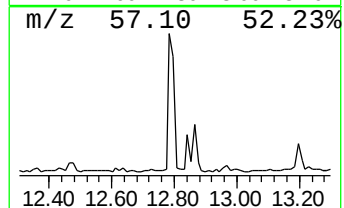
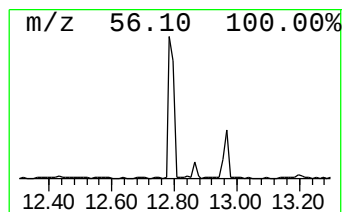
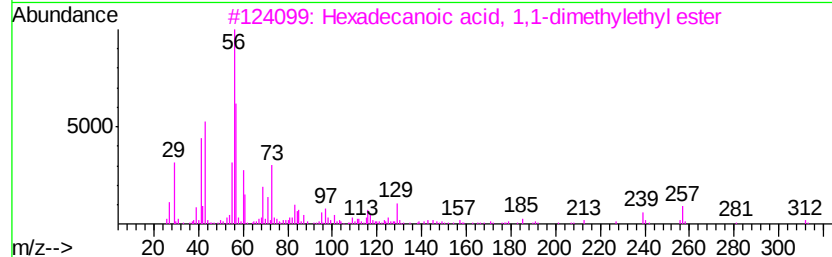
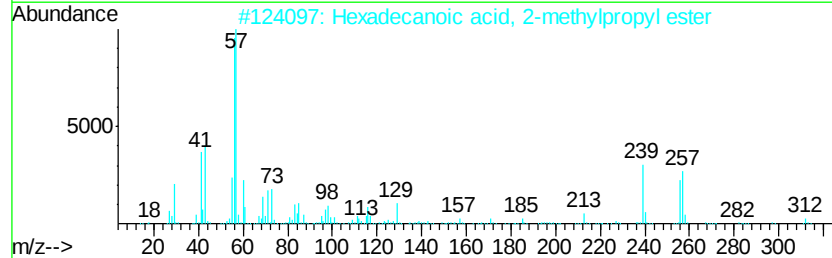
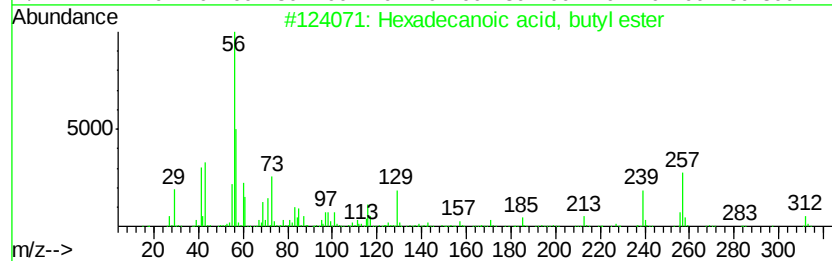
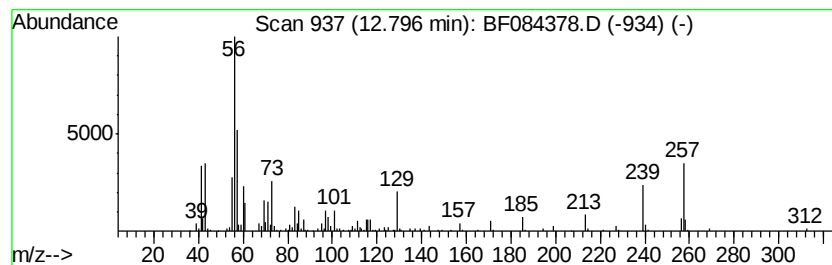
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	5.97 ng	408029	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	94
2		Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	59
3		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	50
4		1-Piperidinyloxy, 4-(hydroxyimin...	185	C9H17N2O2	003229-75-2	27
5		2,2-Dimethyl-1,3-butanediol	118	C6H14O2	000076-35-7	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011116\
Data File : BF084378.D
Acq On : 11 Jan 2016 14:30
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Misc :
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Instrument :
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ClientSampleId :
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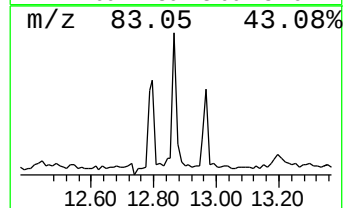
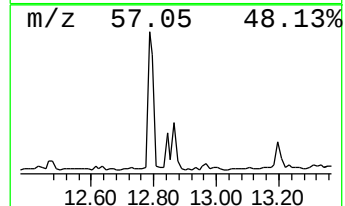
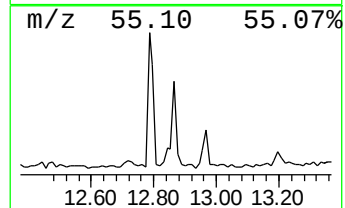
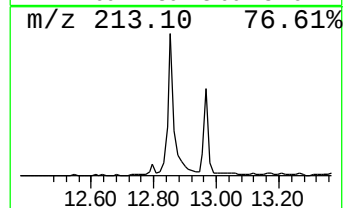
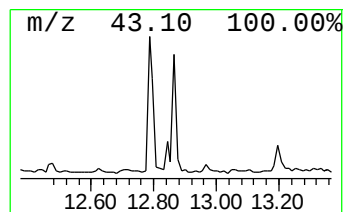
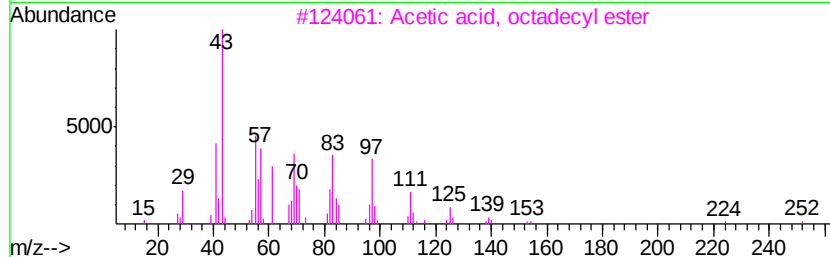
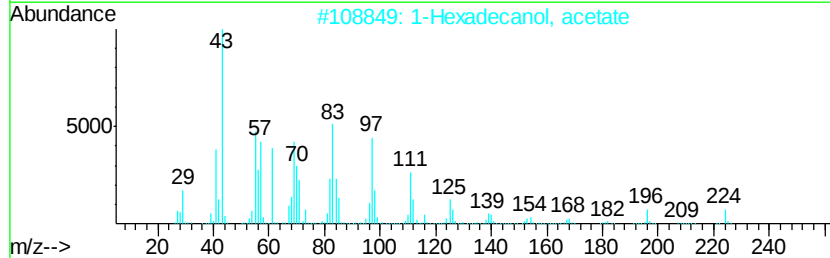
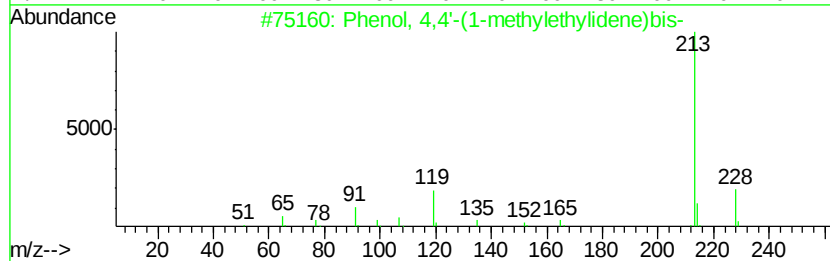
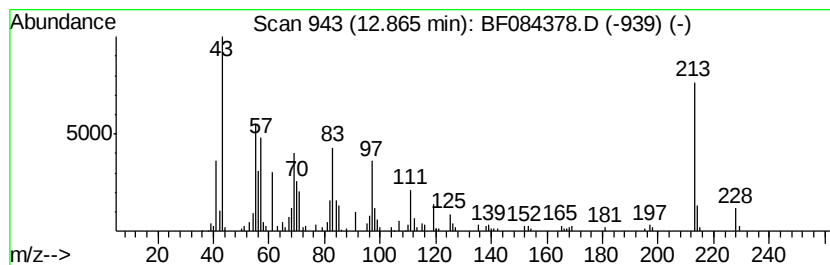
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Phenol, 4,4'-(1-methylethyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.87	4.87 ng	332917	Chrysene-d12	14.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	84
2		1-Hexadecanol, acetate	284	C18H36O2	000629-70-9	50
3		Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	45
4		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	42
5		5-Eicosene, (E)-	280	C20H40	074685-30-6	42



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011116\
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Acq On : 11 Jan 2016 14:30
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Sample : H1043-16
Misc :
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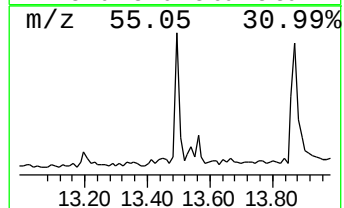
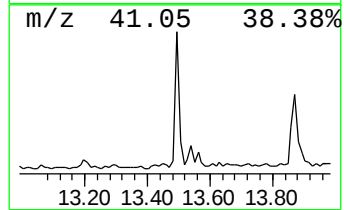
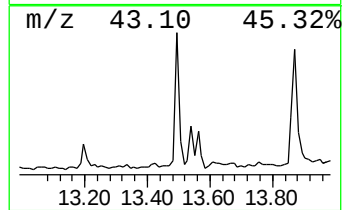
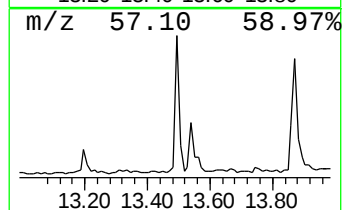
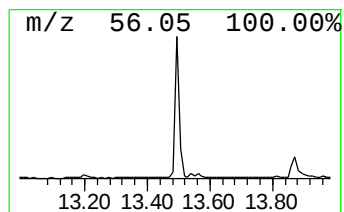
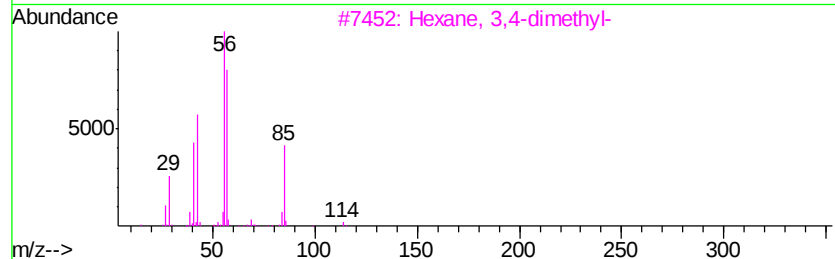
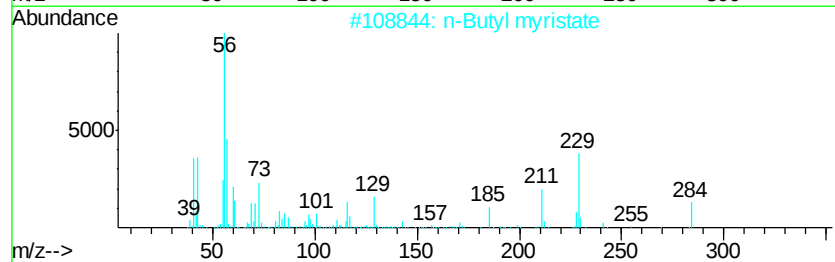
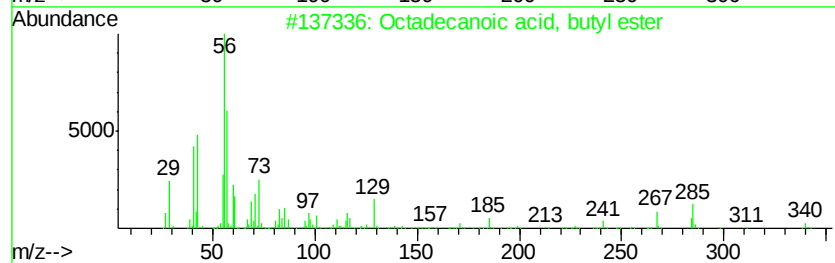
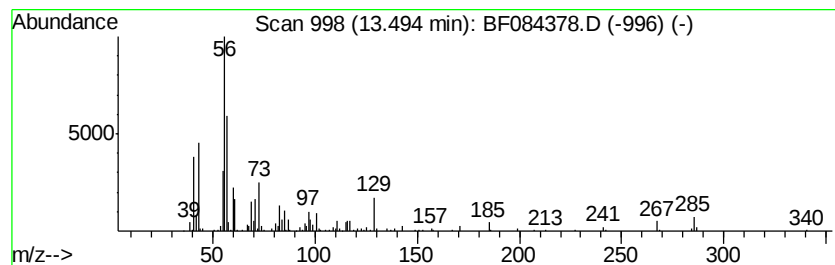
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.49	4.29 ng	293264	Chrysene-d12	14.02		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2		n-Butyl myristate	284	C18H36O2	000110-36-1	90
3		Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	38
4		Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	38
5		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011116\
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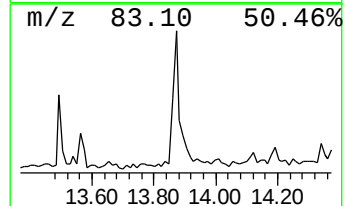
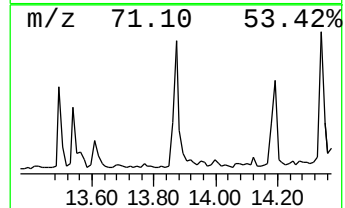
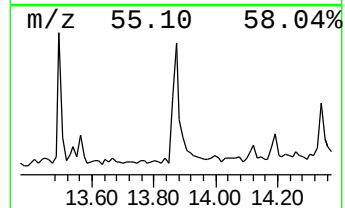
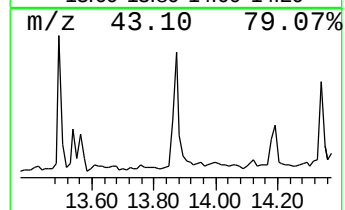
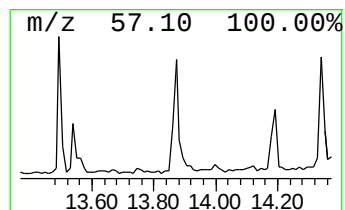
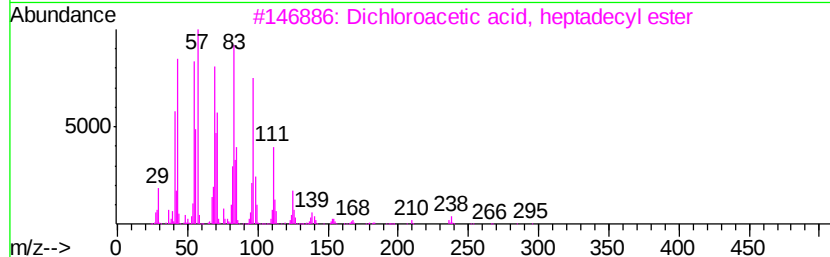
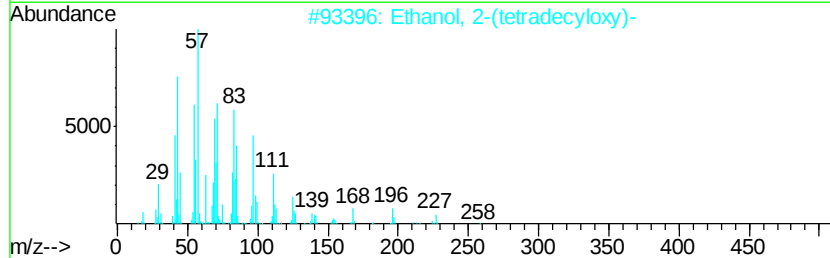
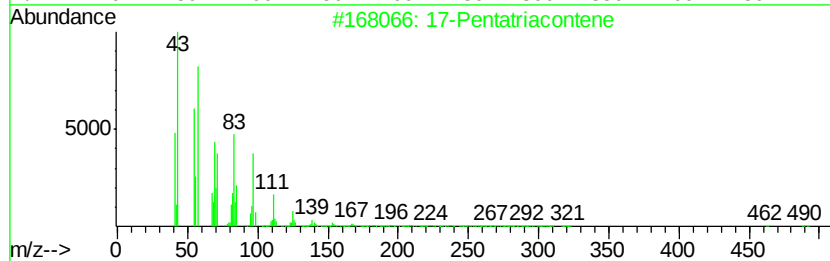
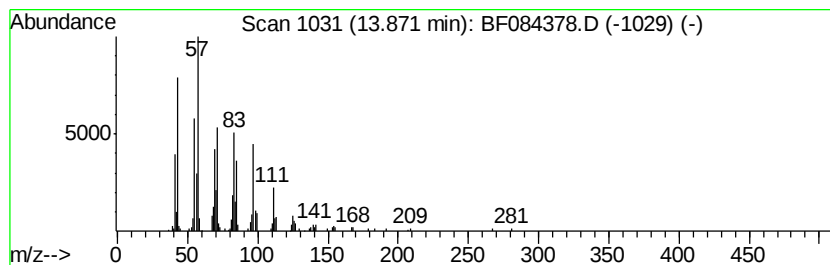
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 17-Pentatriacontene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	4.40 ng	300422	Chrysene-d12	14.02
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		17-Pentatriacontene	491 C35H70	006971-40-0 90
2		Ethanol, 2-(tetradecyloxy)-	258 C16H34O2	002136-70-1 80
3		Dichloroacetic acid, heptadecyl ...	366 C19H36Cl2O2	1000282-98-2 74
4		1-Decanol, 2-hexyl-	242 C16H34O	002425-77-6 74
5		Pentafluoropropionic acid, hepta...	402 C20H35F5O2	1000283-04-2 72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011116\
Data File : BF084378.D
Acq On : 11 Jan 2016 14:30
Operator : SJ/UM
Sample : H1043-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3COMP

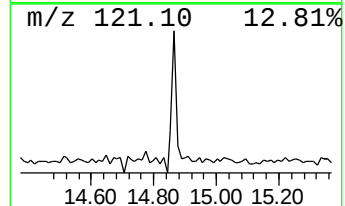
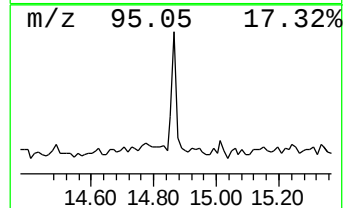
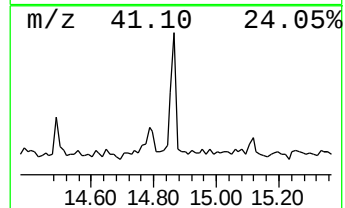
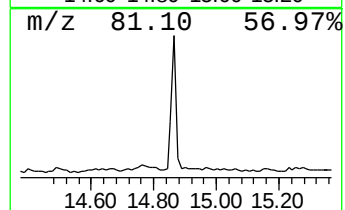
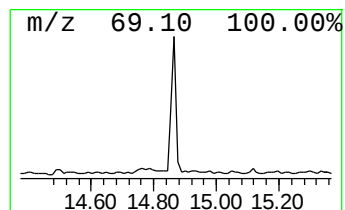
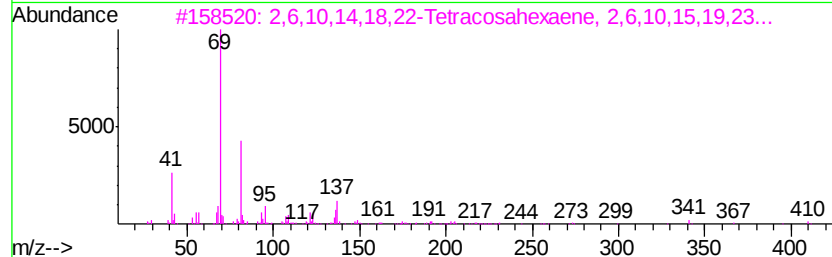
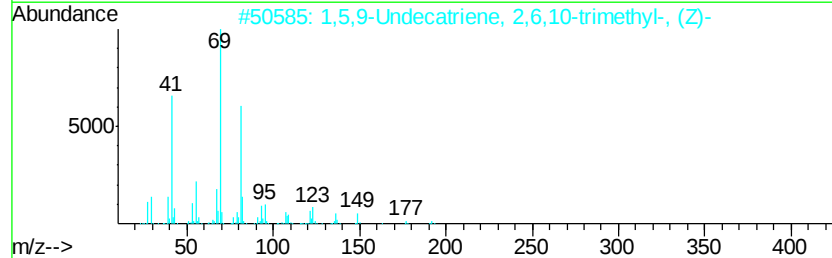
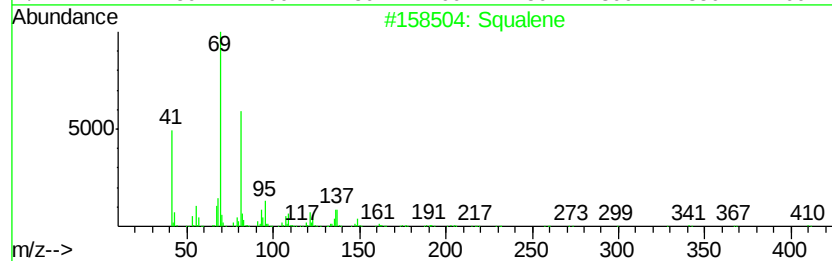
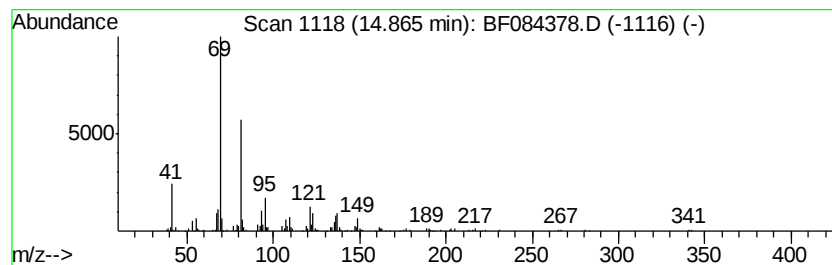
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	3.26 ng	194391	Perylene-d12	15.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	90
2		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	78
3		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	72
4		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	000106-28-5	72
5		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011116\
 Data File : BF084378.D
 Acq On : 11 Jan 2016 14:30
 Operator : SJ/UM
 Sample : H1043-16
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-3COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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...	5.05	28.5	ng	2319540	1	6.85	1626680	20.0
unknown6.64	6.64	106.2	ng	8635400	1	6.85	1626680	20.0
2-Ethylhexyl merc...	9.49	2.6	ng	280138	3	9.89	2170340	20.0
Hexadecane	9.82	2.0	ng	218174	3	9.89	2170340	20.0
Tetradecane	10.33	3.3	ng	361312	3	9.89	2170340	20.0
Pentadecane, 2,6,...	10.54	2.1	ng	226533	3	9.89	2170340	20.0
Benzenesulfonamid...	10.80	9.7	ng	952785	4	11.38	1962920	20.0
Tetracosane	11.25	2.0	ng	201004	4	11.38	1962920	20.0
Hexadecanoic acid...	12.80	6.0	ng	408029	5	14.02	1366350	20.0
Phenol, 4,4'-(1-m...	12.87	4.9	ng	332917	5	14.02	1366350	20.0
Octadecanoic acid...	13.49	4.3	ng	293264	5	14.02	1366350	20.0
17-Pentatriacontene	13.87	4.4	ng	300422	5	14.02	1366350	20.0
Squalene	14.87	3.3	ng	194391	6	15.45	1192760	20.0