

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042916\
 Data File : BF086492.D
 Acq On : 29 Apr 2016 15:13
 Operator : UM/SJ
 Sample : H2685-02
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 26WARD-2A-CS-10(6-12FTBGS)

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-BF042716.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	3.424	114	117	127	rVB	29638	66801	1.27%	0.132%
2	4.281	190	192	196	rBV	60067	95804	1.82%	0.190%
3	4.967	249	252	259	rBV	196288	305056	5.79%	0.604%
4	5.378	285	288	290	rBV	4305173	4816604	91.39%	9.543%
5	5.447	293	294	303	rVB	39676	70581	1.34%	0.140%
6	6.419	375	379	381	rBV	4103619	4911484	93.19%	9.731%
7	6.544	387	390	393	rBV	4438659	4742948	89.99%	9.398%
8	6.773	408	410	415	rBV	1070575	1050355	19.93%	2.081%
9	6.933	421	424	426	rBV	3885257	3862788	73.29%	7.654%
10	7.344	456	460	462	rBV	2994281	3470422	65.85%	6.876%
11	7.436	466	468	476	rVV	55007	156030	2.96%	0.309%
12	8.064	520	523	525	rBV	1079884	1377321	26.13%	2.729%
13	8.179	532	533	544	rVB	34142	63826	1.21%	0.126%
14	8.602	567	570	572	rVB2	94075	112995	2.14%	0.224%
15	8.922	595	598	604	rVB2	99044	156350	2.97%	0.310%
16	9.139	614	617	620	rBV	3942225	5270273	100.00%	10.442%
17	9.539	649	652	654	rBV	794569	801158	15.20%	1.587%
18	9.756	668	671	673	rBV	92947	81596	1.55%	0.162%
19	9.813	673	676	678	rBV	1661033	1577109	29.92%	3.125%
20	9.848	678	679	681	rVB	80755	63945	1.21%	0.127%
21	10.259	710	715	716	rBV	134807	187320	3.55%	0.371%
22	10.362	722	724	727	rBV	47108	62481	1.19%	0.124%
23	10.476	730	734	735	rBV	66778	100234	1.90%	0.199%
24	10.602	742	745	748	rBV	3012293	3390342	64.33%	6.718%
25	10.728	754	756	763	rVB	228876	307227	5.83%	0.609%
26	10.922	768	773	777	rBV4	31413	90797	1.72%	0.180%
27	11.173	793	795	796	rBV	117489	97596	1.85%	0.193%
28	11.299	803	806	810	rBV2	1018126	1943829	36.88%	3.851%
29	11.368	810	812	817	rVB	113271	165293	3.14%	0.328%
30	11.528	823	826	830	rBV3	47382	86375	1.64%	0.171%
31	11.836	850	853	854	rVV2	80547	143728	2.73%	0.285%
32	11.905	857	859	864	rVB2	95469	154194	2.93%	0.306%
33	12.088	872	875	876	rBV	94671	107185	2.03%	0.212%
34	12.351	895	898	901	rBV2	157279	271787	5.16%	0.539%

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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-BF042716.M
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35	12.499	909	911	914	rBV	615313	577700	10.96%	1.145%
36	12.648	921	924	928	rVB3	24536	54463	1.03%	0.108%
37	12.728	928	931	933	rBV	502665	578570	10.98%	1.146%
38	12.785	933	936	940	rVB3	32969	65506	1.24%	0.130%
39	12.888	942	945	947	rBV	3448991	4704410	89.26%	9.321%
40	13.059	956	960	962	rVB2	43164	83354	1.58%	0.165%
41	13.116	962	965	967	rBV3	29816	61143	1.16%	0.121%
42	13.459	989	995	1000	rBV5	29114	84926	1.61%	0.168%
43	13.665	1011	1013	1015	rBV2	27003	53526	1.02%	0.106%
44	13.779	1021	1023	1027	rBV2	164571	220103	4.18%	0.436%
45	13.916	1032	1035	1042	rBV	810780	1525632	28.95%	3.023%
46	14.099	1049	1051	1061	rVB4	27511	75841	1.44%	0.150%
47	14.408	1076	1078	1084	rBV4	32648	76319	1.45%	0.151%
48	14.682	1099	1102	1107	rBV	181228	281238	5.34%	0.557%
49	14.762	1107	1109	1112	rVB	77723	114171	2.17%	0.226%
50	14.922	1121	1123	1129	rBV	109258	275761	5.23%	0.546%
51	15.197	1145	1147	1150	rVV	57191	93009	1.76%	0.184%
52	15.265	1150	1153	1155	rVV	65252	102330	1.94%	0.203%
53	15.322	1155	1158	1169	rVB	621091	963642	18.28%	1.909%
54	16.660	1272	1275	1276	rBV	29662	61677	1.17%	0.122%
55	16.705	1276	1279	1282	rVB	81736	147406	2.80%	0.292%
56	17.048	1306	1309	1317	rBV	41315	107493	2.04%	0.213%

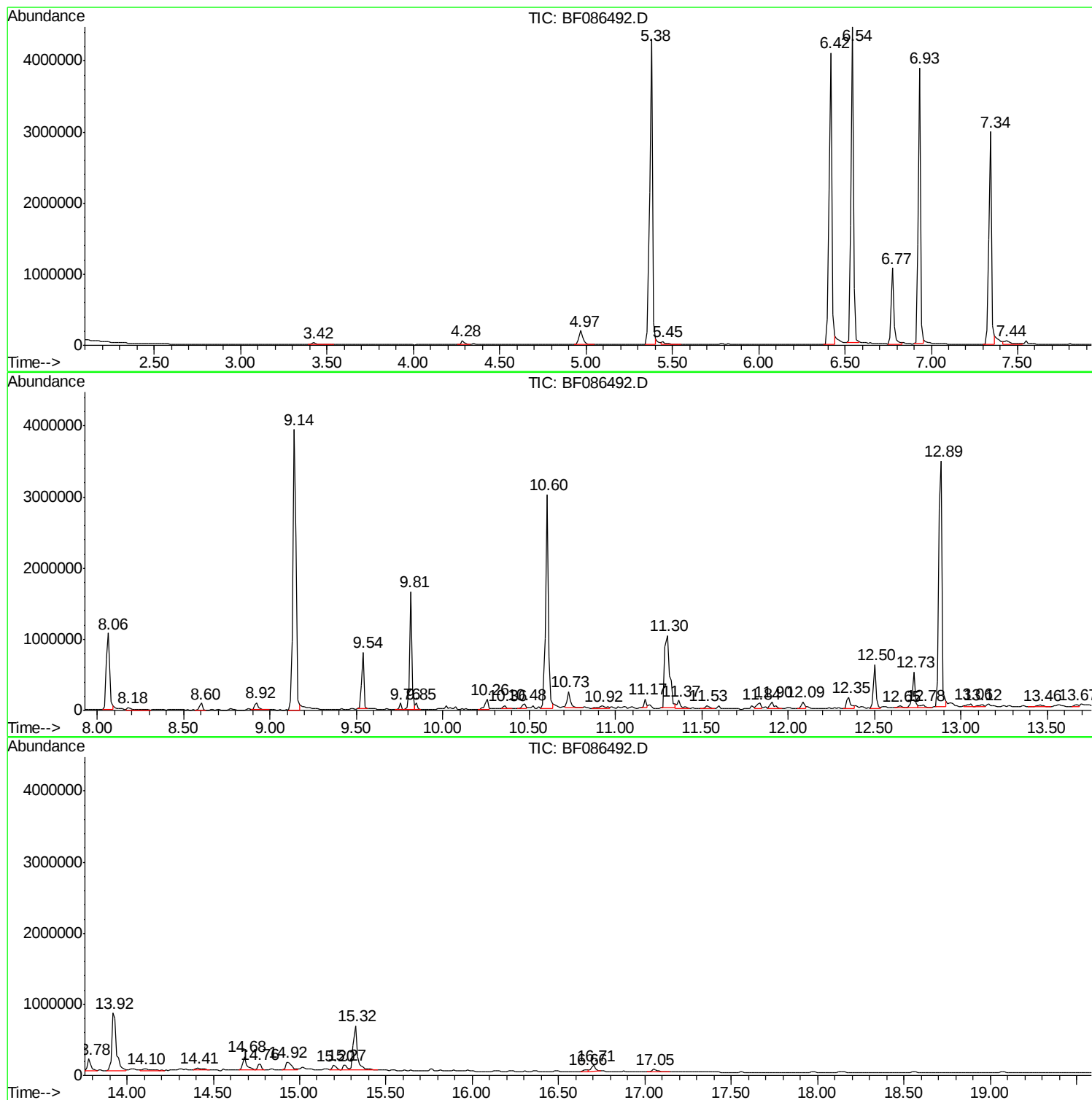
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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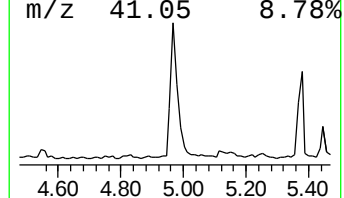
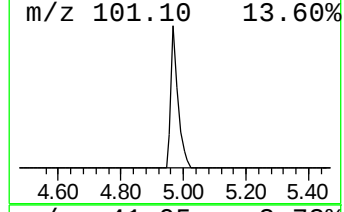
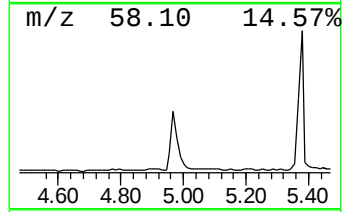
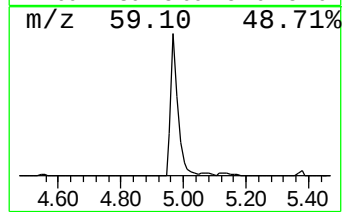
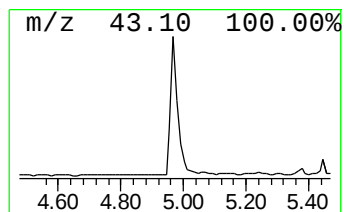
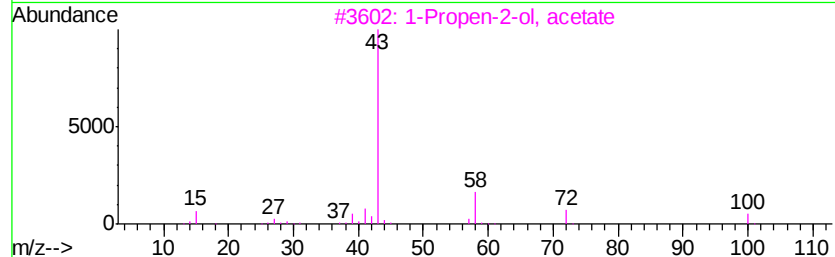
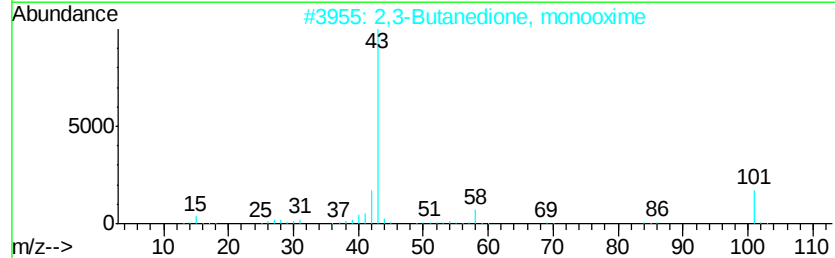
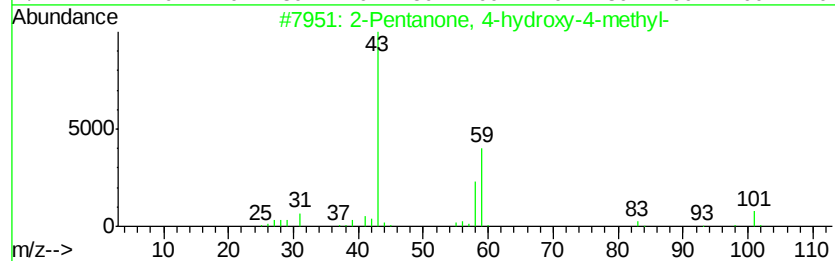
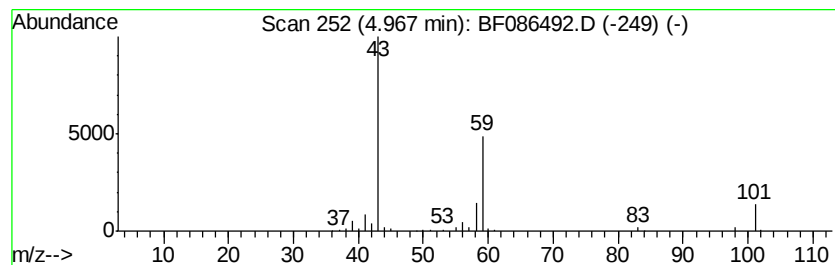
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	5.81 ng	305056	1,4-Dichlorobenzene-d4	6.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	Diacetamide	101	C4H7NO2	000625-77-4	9		
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9		



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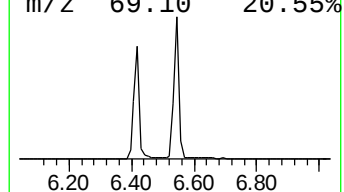
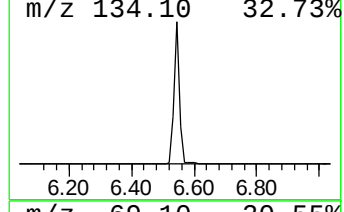
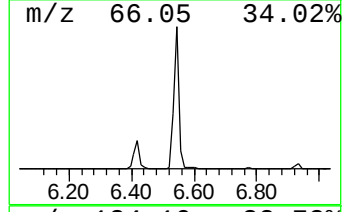
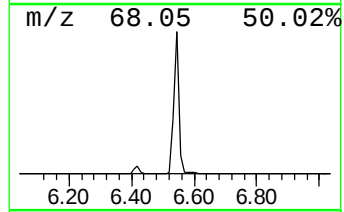
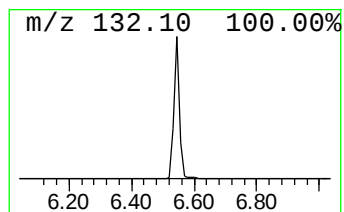
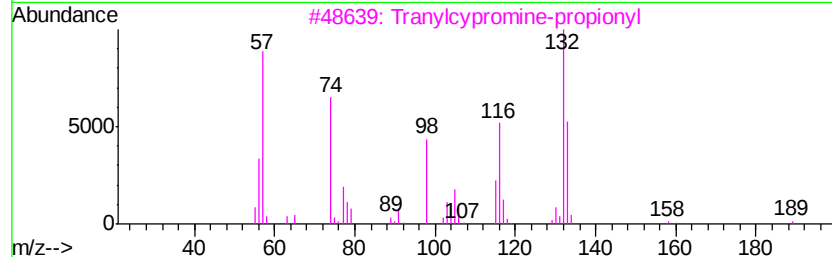
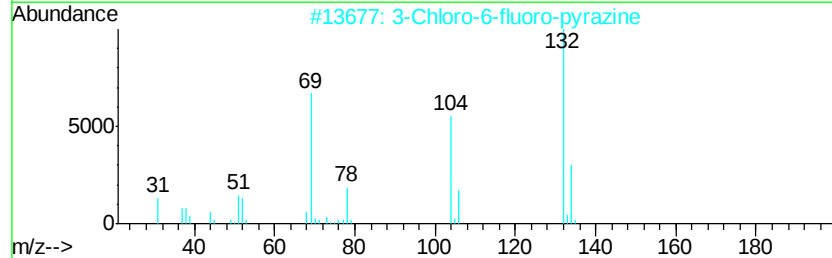
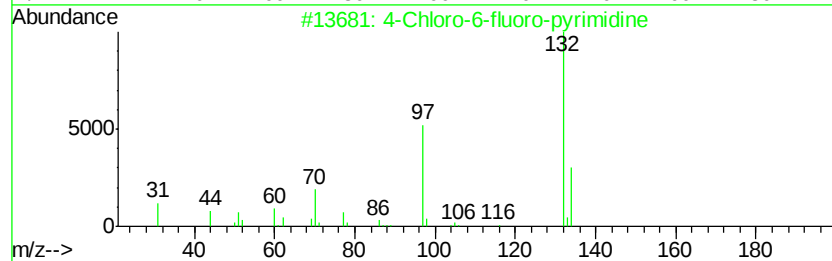
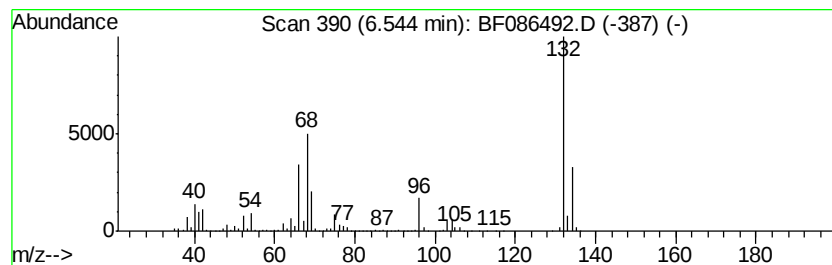
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	90.31 ng	4742950	1,4-Dichlorobenzene-d4	6.77

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		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	22
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16



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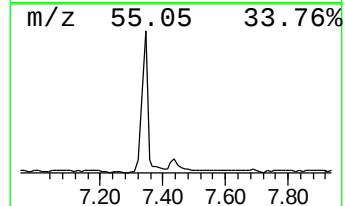
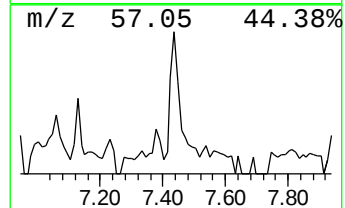
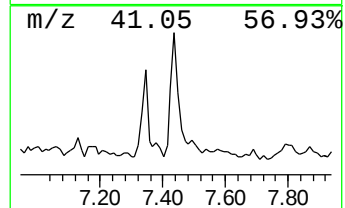
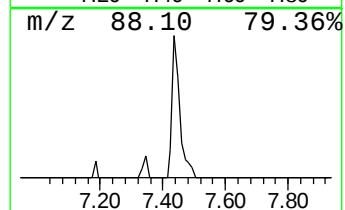
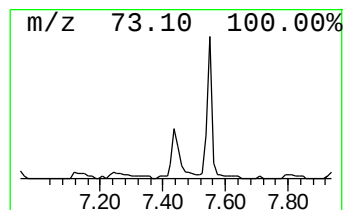
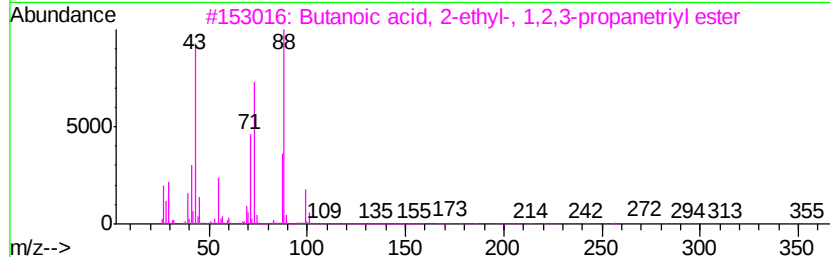
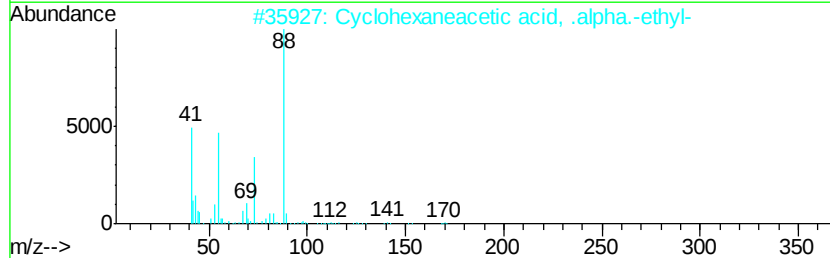
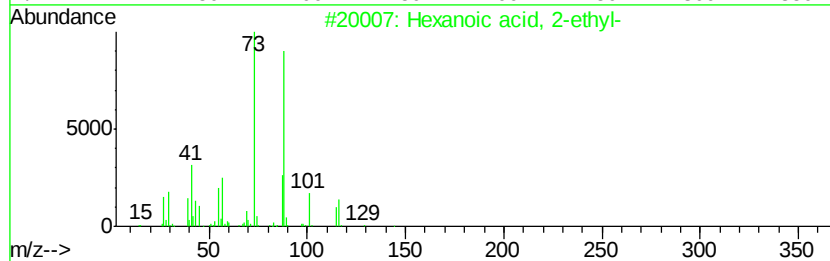
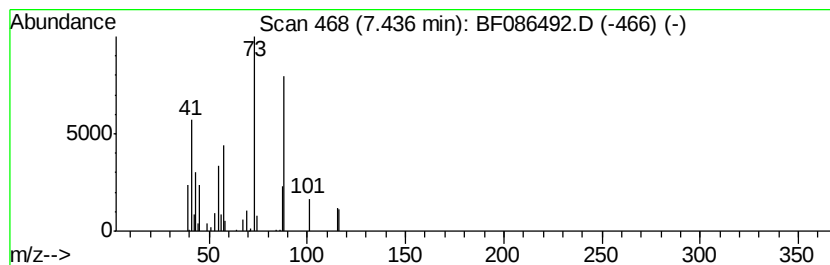
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.44	2.27 ng	156030	Naphthalene-d8	8.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	72
2		Cyclohexaneacetic acid, .alpha.-...	170	C10H18O2	006051-00-9	37
3		Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	36
4		Methyl L-(+)-.beta.-hydroxyisobu...	118	C5H10O3	080657-57-4	28
5		Propanoic acid, 3-hydroxy-2-meth...	118	C5H10O3	042998-03-8	28



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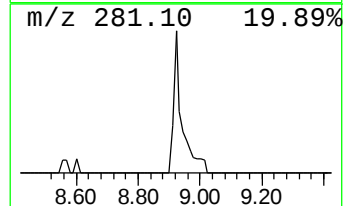
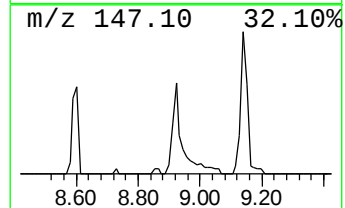
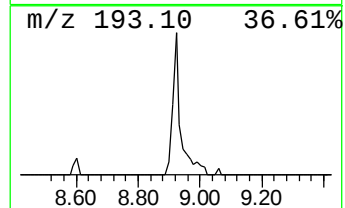
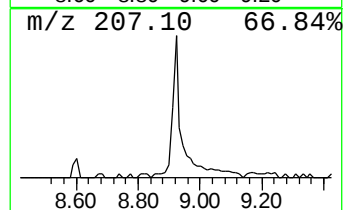
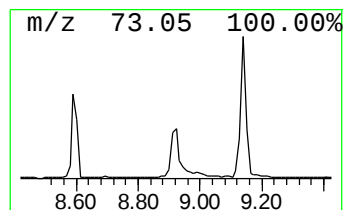
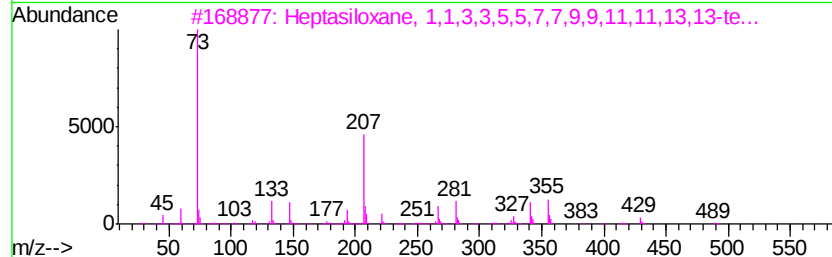
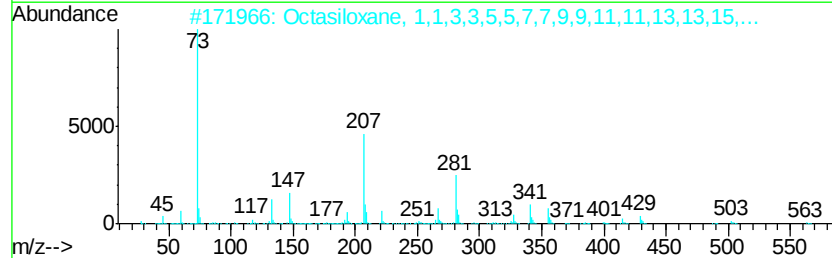
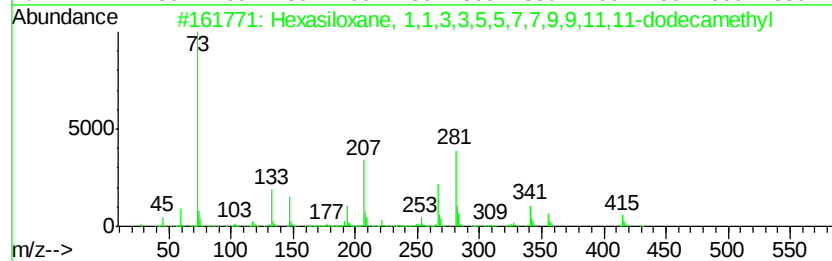
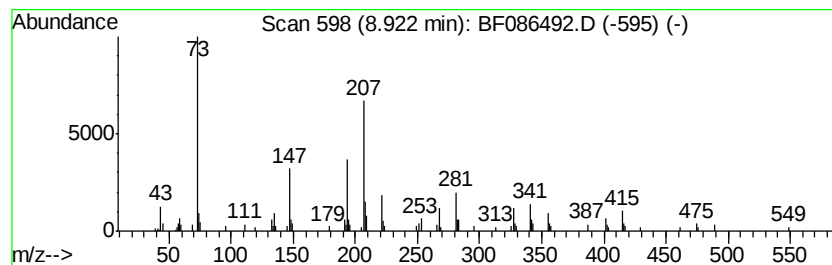
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Peak Number 5 Hexasiloxane, 1,1,3,3,5,5,7... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.92	2.27 ng	156350	Naphthalene-d8	8.06	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexasiloxane, 1,1,3,3,5,5,7,7,9,...	430	C12H38O5Si6	000995-82-4	50
2	Octasiloxane, 1,1,3,3,5,5,7,7,9,...	578	C16H50O7Si8	019095-24-0	49
3	Heptasiloxane, 1,1,3,3,5,5,7,7,9...	504	C14H44O6Si7	019095-23-9	47
4	3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	38
5	5,5'-Di(ethoxycarbonyl)-3,3'-dim...	402	C23H34N2O4	102586-97-0	35



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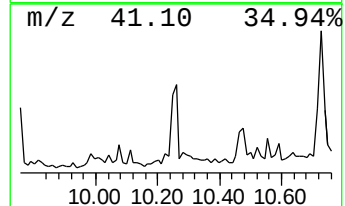
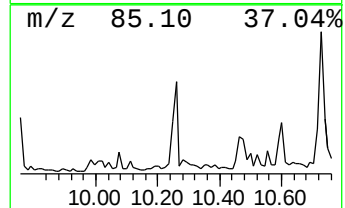
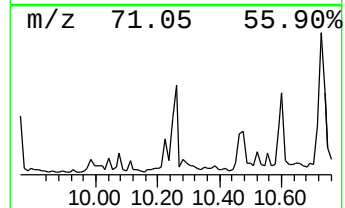
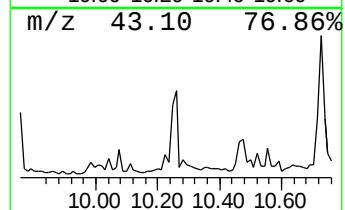
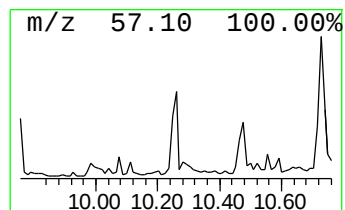
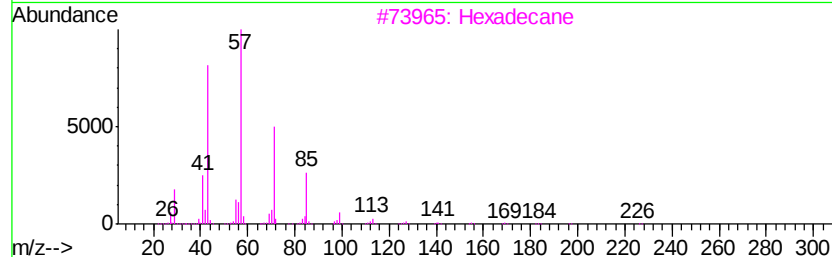
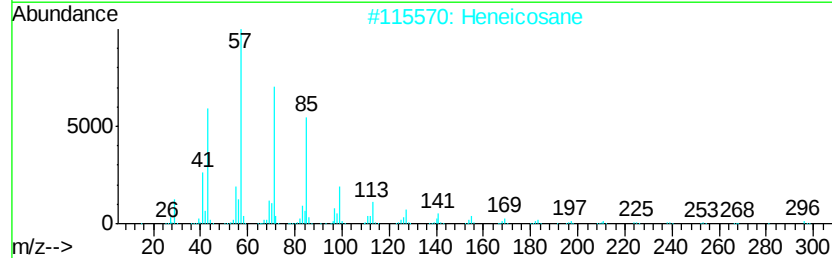
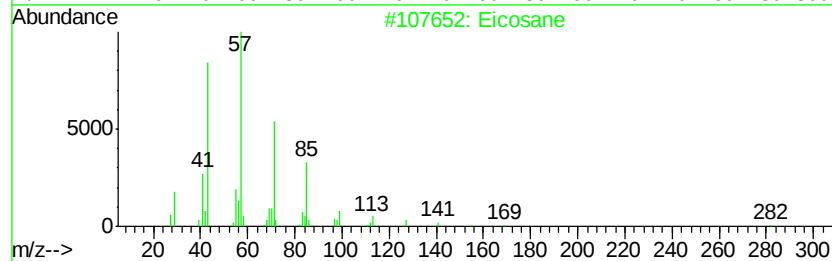
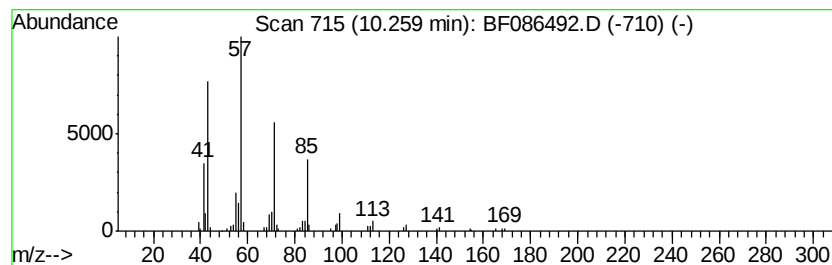
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.26	2.38 ng	187320	Acenaphthene-d10	9.81

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Heneicosane		296	C21H44	000629-94-7	90
3	Hexadecane		226	C16H34	000544-76-3	90
4	Tetracosane		338	C24H50	000646-31-1	90
5	Tridecane		184	C13H28	000629-50-5	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042916\
Data File : BF086492.D
Acq On : 29 Apr 2016 15:13
Operator : UM/SJ
Sample : H2685-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
26WARD-2A-CS-10(6-12FTBGS)

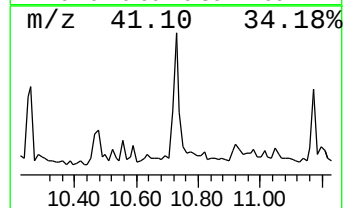
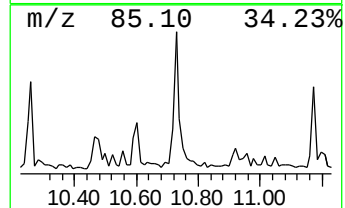
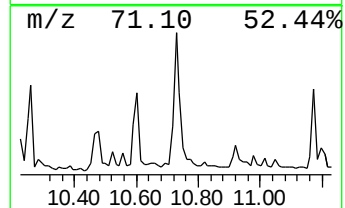
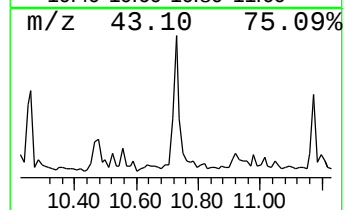
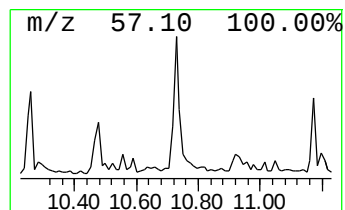
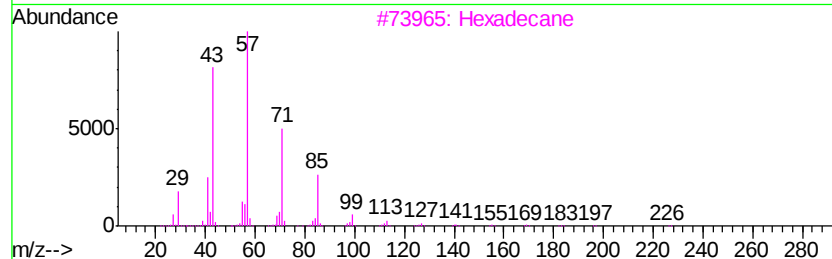
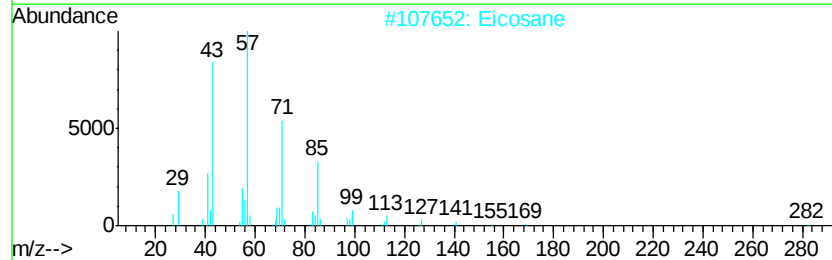
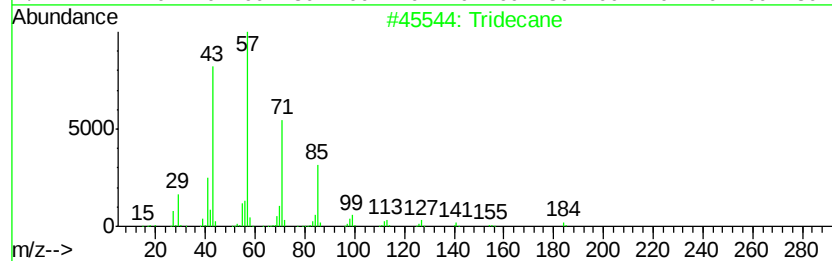
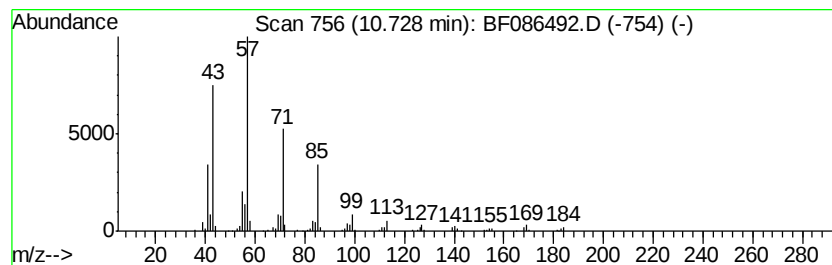
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tridecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.73	3.16 ng	307227	Phenanthrene-d10	11.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecane	184	C13H28	000629-50-5	96
2		Eicosane	282	C20H42	000112-95-8	91
3		Hexadecane	226	C16H34	000544-76-3	91
4		Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	90
5		Nonadecane	268	C19H40	000629-92-5	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042916\
Data File : BF086492.D
Acq On : 29 Apr 2016 15:13
Operator : UM/SJ
Sample : H2685-02
Misc :
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Instrument :
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ClientSampleId :
26WARD-2A-CS-10(6-12FTBGS)

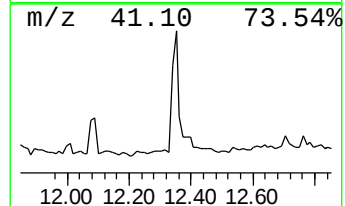
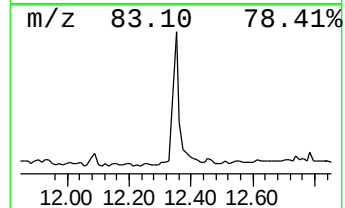
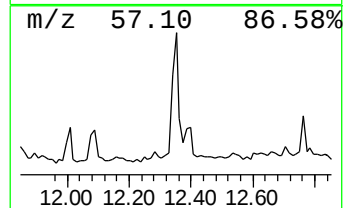
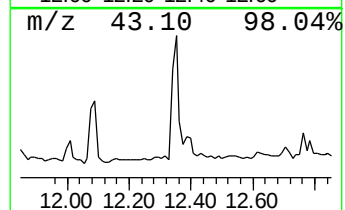
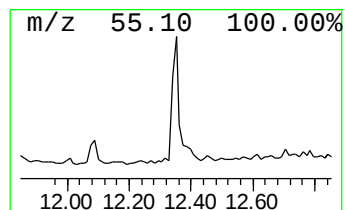
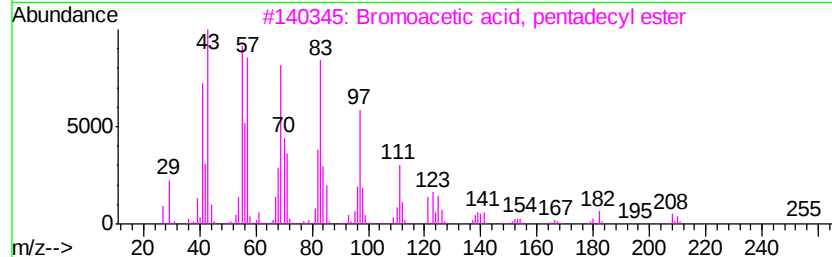
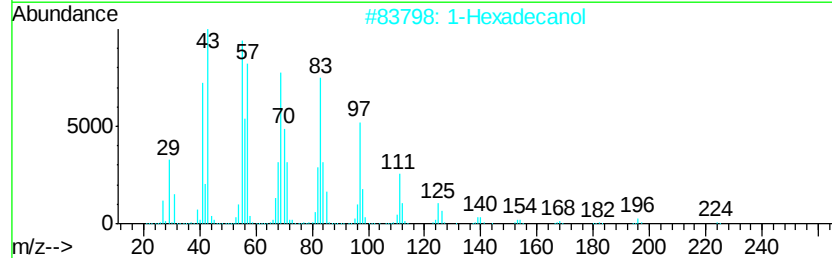
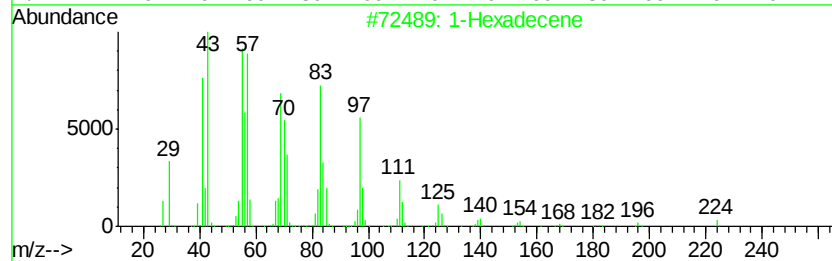
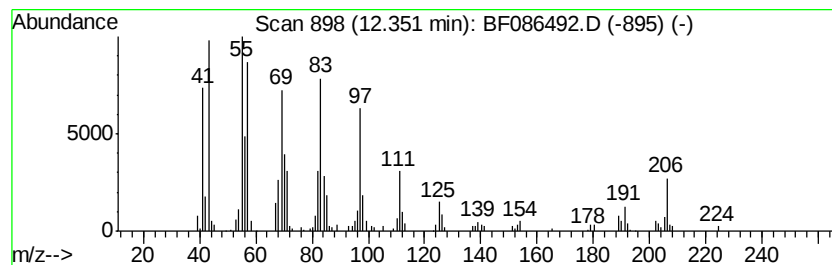
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Hexadecene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.35	2.80 ng	271787	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecene	224	C16H32	000629-73-2	95
2	1-Hexadecanol	242	C16H34O	036653-82-4	93
3	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	91
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	87
5	1-Octadecanol	270	C18H38O	000112-92-5	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042916\
Data File : BF086492.D
Acq On : 29 Apr 2016 15:13
Operator : UM/SJ
Sample : H2685-02
Misc :
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Instrument :
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ClientSampleId :
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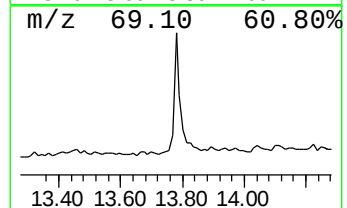
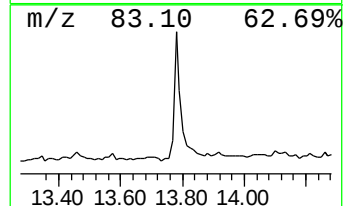
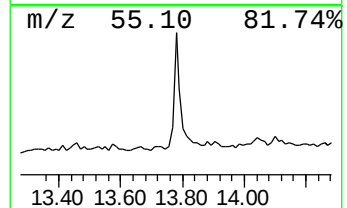
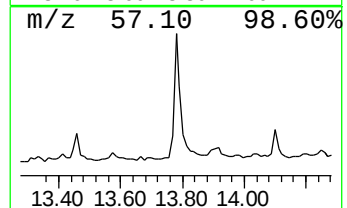
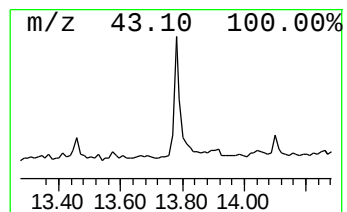
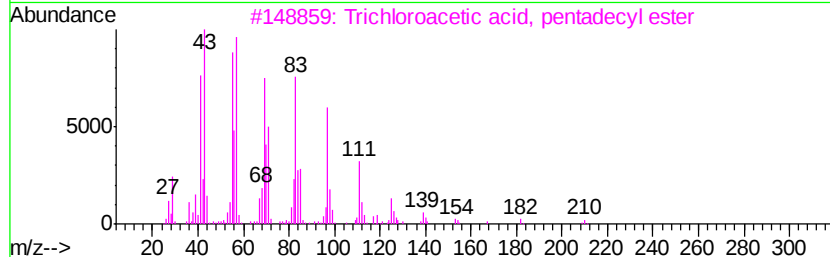
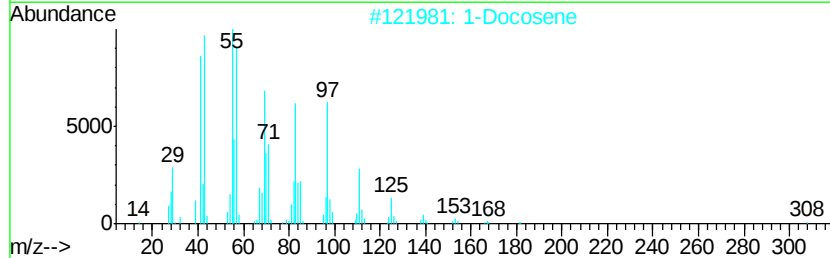
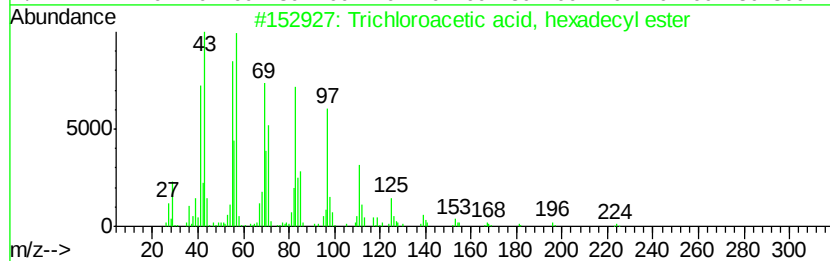
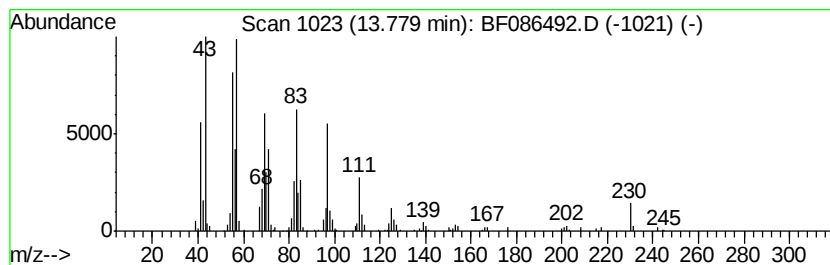
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Trichloroacetic acid, hexad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.78	2.89 ng	220103	Chrysene-d12	13.93

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2			1-Docosene	308	C22H44	001599-67-3	93
3			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4			Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	87
5			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042916\
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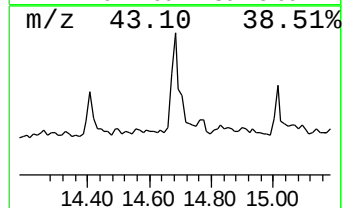
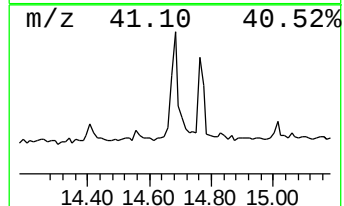
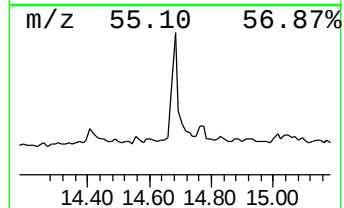
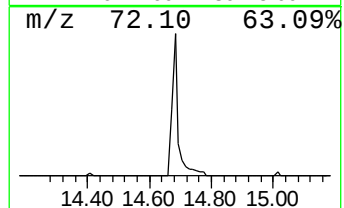
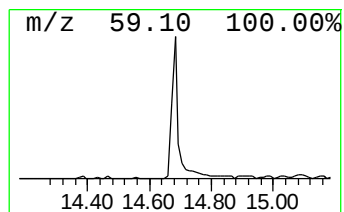
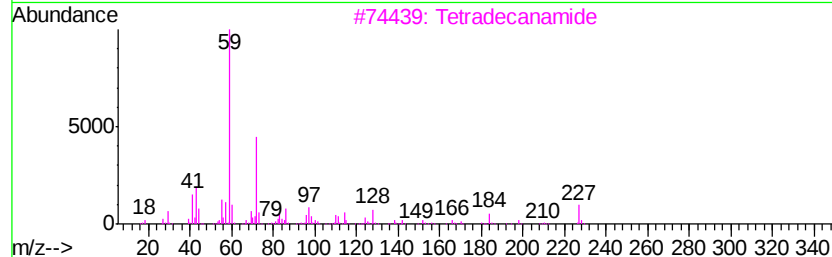
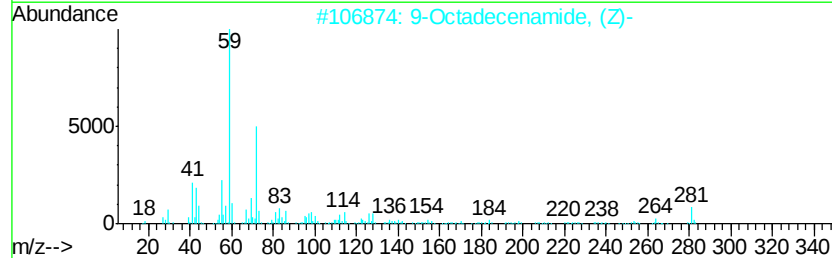
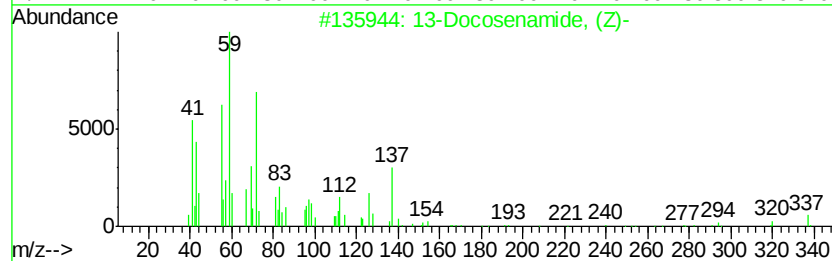
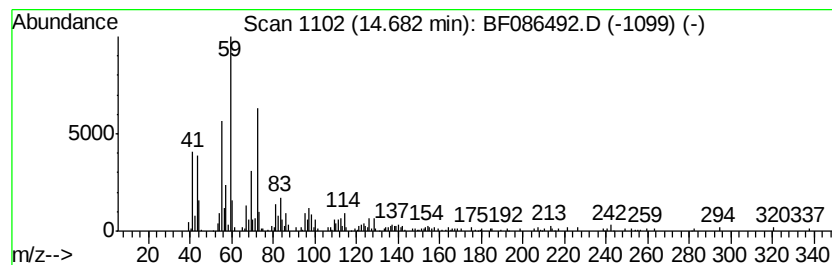
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ClientSampleId :
26WARD-2A-CS-10(6-12FTBGS)

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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 13-Docosenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.68	5.84 ng	281238	Perylene-d12	15.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	90
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
3	Tetradecanamide	227	C14H29NO	000638-58-4	64
4	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	59
5	7-Nonenamide	155	C9H17NO	090949-53-4	58



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042916\
Data File : BF086492.D
Acq On : 29 Apr 2016 15:13
Operator : UM/SJ
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Misc :
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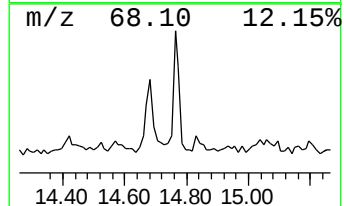
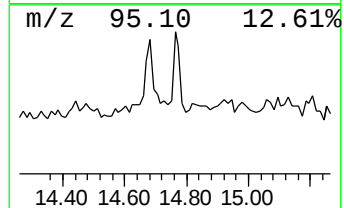
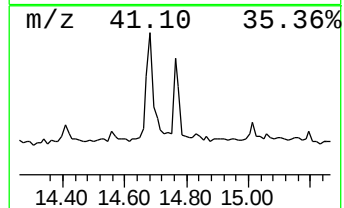
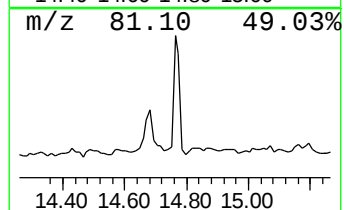
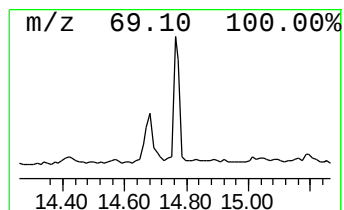
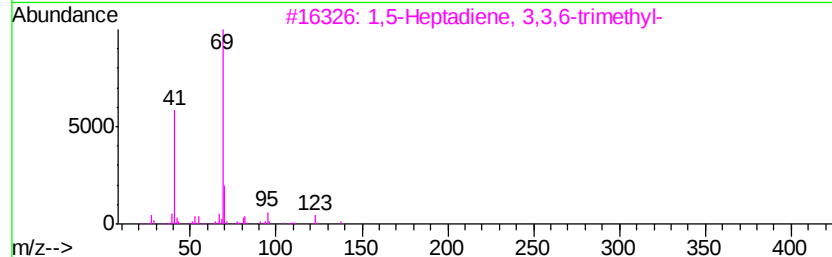
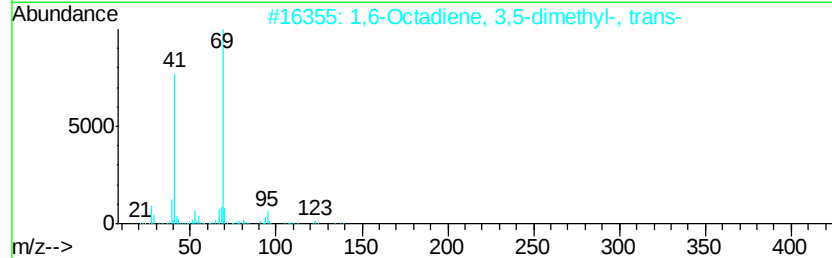
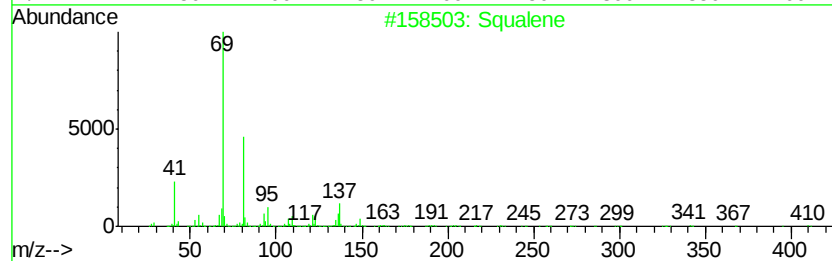
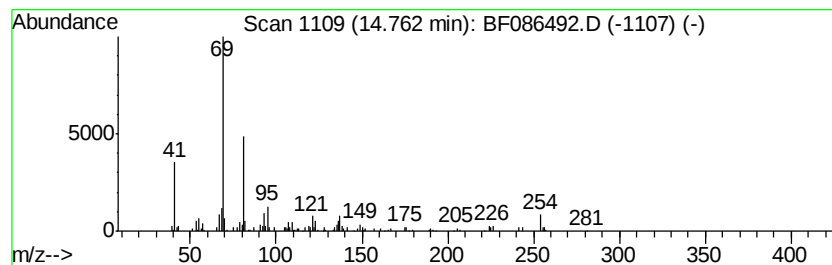
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.76	2.37 ng	114171	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	87
2		1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	59
3		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	59
4		2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	53
5		1,5-Heptadiene, 3,4-dimethyl-	124	C9H16	1000061-77-9	53



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042916\
Data File : BF086492.D
Acq On : 29 Apr 2016 15:13
Operator : UM/SJ
Sample : H2685-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
26WARD-2A-CS-10(6-12FTBGS)

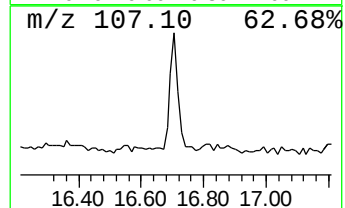
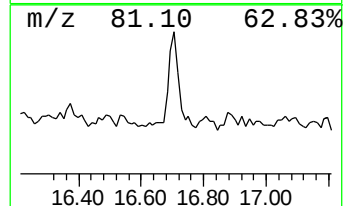
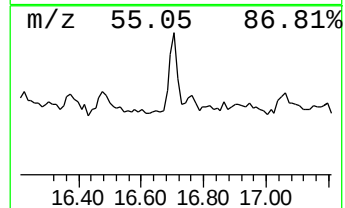
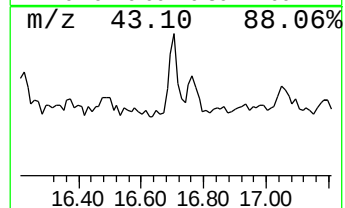
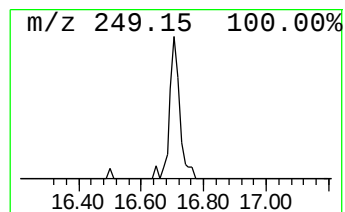
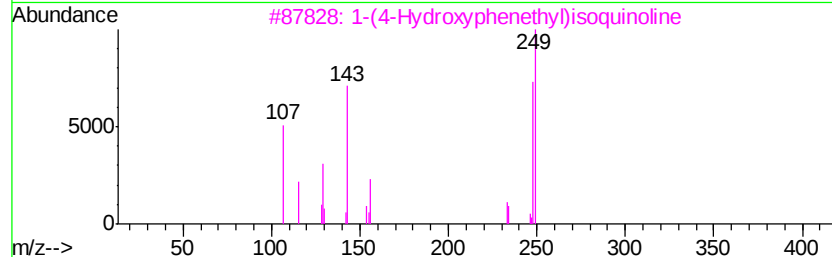
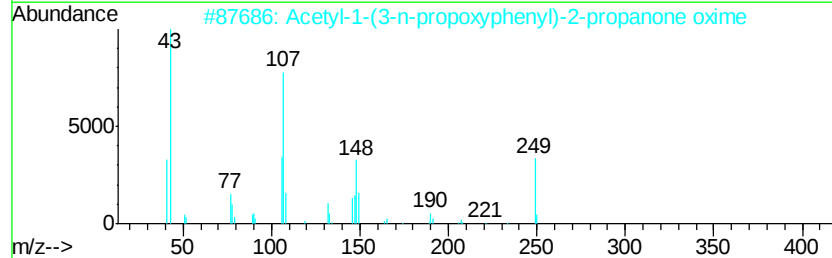
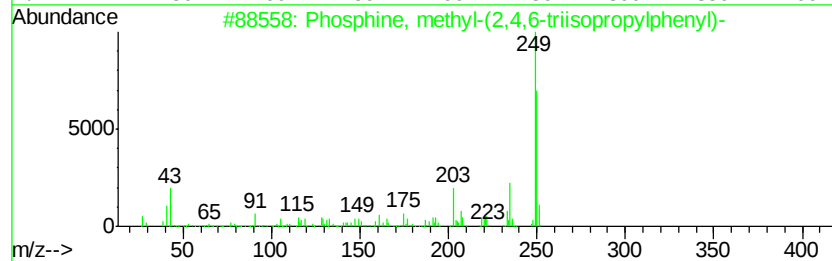
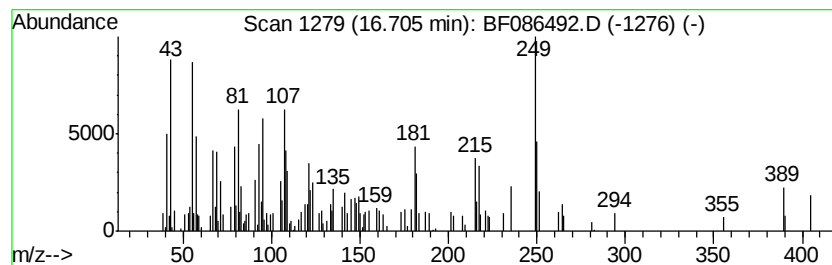
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown16.71 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.71	3.06 ng	147406	Perylene-d12	15.32

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phosphine, methyl-(2,4,6-triisop...	250	C16H27P	158748-69-7	30
2			Acetyl-1-(3-n-propoxyphenyl)-2-p...	249	C14H19NO3	1000122-90-2	27
3			1-(4-Hydroxyphenethyl)isoquinoline	249	C17H15NO	078744-89-5	22
4			1-Ethanone, 1-{2-[(3,3-dimethyl-...	292	C16H24N2OS	077109-20-7	16
5			7H-Benzo(c)phenothiazine	249	C16H11NS	000226-06-2	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042916\
Data File : BF086492.D
Acq On : 29 Apr 2016 15:13
Operator : UM/SJ
Sample : H2685-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
26WARD-2A-CS-10(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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...	4.97	5.8	ng	305056	1	6.77	1050360	20.0
unknown6.54	6.54	90.3	ng	4742950	1	6.77	1050360	20.0
Hexanoic acid, 2-...	7.44	2.3	ng	156030	2	8.06	1377320	20.0
Hexasiloxane, 1,1...	8.92	2.3	ng	156350	2	8.06	1377320	20.0
Eicosane	10.26	2.4	ng	187320	3	9.81	1577110	20.0
Tridecane	10.73	3.2	ng	307227	4	11.30	1943830	20.0
1-Hexadecene	12.35	2.8	ng	271787	4	11.30	1943830	20.0
Trichloroacetic a...	13.78	2.9	ng	220103	5	13.93	1525630	20.0
13-Docosenamide, ...	14.68	5.8	ng	281238	6	15.32	963642	20.0
Squalene	14.76	2.4	ng	114171	6	15.32	963642	20.0
unknown16.71	16.71	3.1	ng	147406	6	15.32	963642	20.0