

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050916\
 Data File : BF086835.D
 Acq On : 9 May 2016 22:05
 Operator : UM/SJ
 Sample : H2895-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP1-6-9FT

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-BF050916.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	4.144	177	180	193	rBV	173691	325247	5.80%	0.633%
2	4.647	222	224	232	rBV	142643	201876	3.60%	0.393%
3	4.864	241	243	250	rBV	278306	527170	9.40%	1.027%
4	5.298	278	281	283	rBV	5012155	5609674	100.00%	10.924%
5	5.698	314	316	326	rVB	34564	67493	1.20%	0.131%
6	6.350	370	373	376	rBV	4398196	5332163	95.05%	10.384%
7	6.464	381	383	385	rBV	5423719	5317231	94.79%	10.355%
8	6.693	400	403	405	rBV	764309	1058230	18.86%	2.061%
9	6.841	414	416	419	rBV	3473389	3552487	63.33%	6.918%
10	7.264	450	453	455	rBV	3513639	3948583	70.39%	7.689%
11	7.973	513	515	518	rBV	1459019	1422309	25.35%	2.770%
12	9.059	606	610	612	rBV	3928460	4898914	87.33%	9.540%
13	9.459	642	645	647	rBV	443084	597216	10.65%	1.163%
14	9.665	661	663	666	rBV	155406	144375	2.57%	0.281%
15	9.722	666	668	671	rVB	1640032	1598906	28.50%	3.114%
16	10.019	692	694	695	rBV	40518	56981	1.02%	0.111%
17	10.167	704	707	708	rVB	202562	216390	3.86%	0.421%
18	10.385	723	726	729	rBV	80594	133120	2.37%	0.259%
19	10.510	734	737	740	rBV2	2723717	4014173	71.56%	7.817%
20	10.636	746	748	754	rVB	274162	345973	6.17%	0.674%
21	10.830	762	765	769	rBV	35388	81065	1.45%	0.158%
22	11.082	785	787	788	rBV	136501	112565	2.01%	0.219%
23	11.208	795	798	800	rBV	1302922	1670681	29.78%	3.253%
24	11.745	843	845	848	rBV	405013	602897	10.75%	1.174%
25	12.419	903	904	912	rVB	151558	233476	4.16%	0.455%
26	12.522	912	913	916	rVB	59605	69823	1.24%	0.136%
27	12.636	921	923	925	rVB	81714	75476	1.35%	0.147%
28	12.785	933	936	939	rBV	3655972	4108049	73.23%	8.000%
29	13.025	955	957	959	rBV2	75796	84423	1.50%	0.164%
30	13.699	1013	1016	1025	rBV	210804	566005	10.09%	1.102%
31	13.825	1025	1027	1030	rBV	1354363	1490771	26.58%	2.903%
32	14.305	1067	1069	1071	rBV	83520	89964	1.60%	0.175%
33	14.351	1071	1073	1076	rVB3	33765	69373	1.24%	0.135%
34	14.602	1091	1095	1097	rBV2	32184	62335	1.11%	0.121%

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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

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Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.659	1098	1100	1104	rVB3	46231	62070	1.11%	0.121%
36	14.728	1104	1106	1108	rBV	70956	68753	1.23%	0.134%
37	14.831	1113	1115	1119	rVV	39953	79336	1.41%	0.154%
38	14.899	1119	1121	1123	rVV	112661	119224	2.13%	0.232%
39	14.956	1123	1126	1135	rVB2	62265	207843	3.71%	0.405%
40	15.208	1145	1148	1150	rBV	709217	1080907	19.27%	2.105%
41	15.608	1180	1183	1187	rBV	66684	95589	1.70%	0.186%
42	15.711	1189	1192	1196	rVB3	19861	56668	1.01%	0.110%
43	17.002	1302	1305	1311	rBV5	20661	75932	1.35%	0.148%
44	17.151	1311	1318	1323	rVB6	34608	117909	2.10%	0.230%
45	17.448	1341	1344	1352	rVB6	27989	86120	1.54%	0.168%
46	17.871	1376	1381	1387	rVB4	46082	132643	2.36%	0.258%
47	18.683	1443	1452	1454	rBV6	46154	213289	3.80%	0.415%
48	18.751	1454	1458	1466	rVB2	83595	269834	4.81%	0.525%

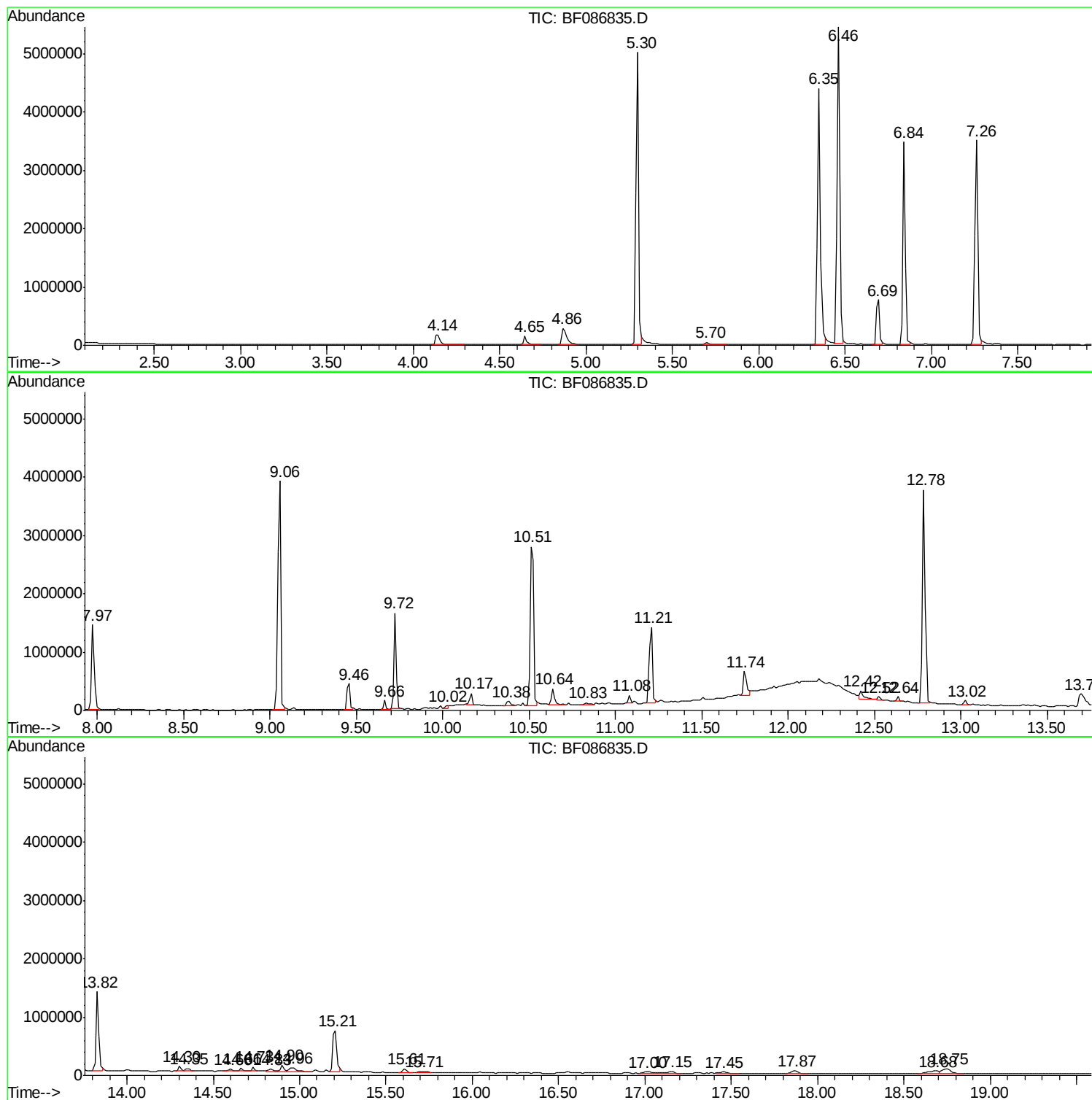
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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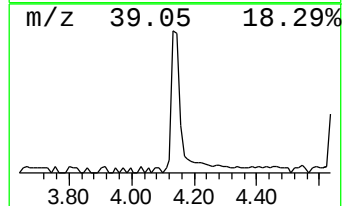
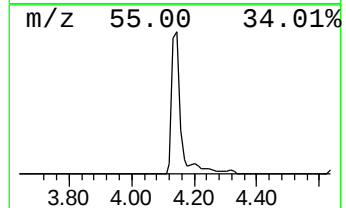
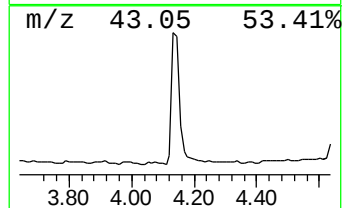
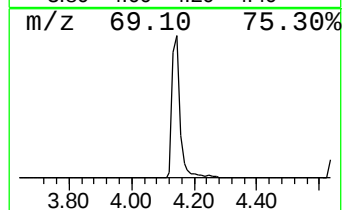
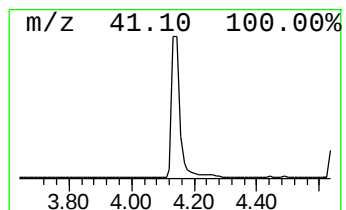
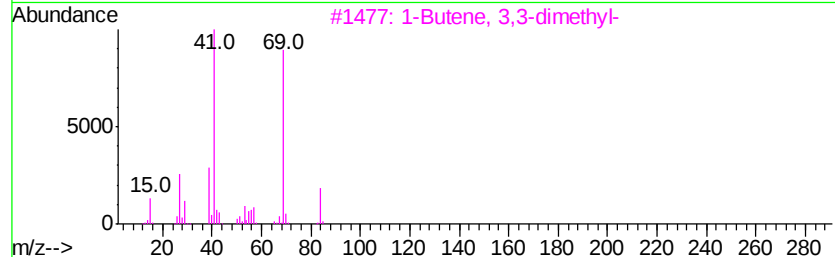
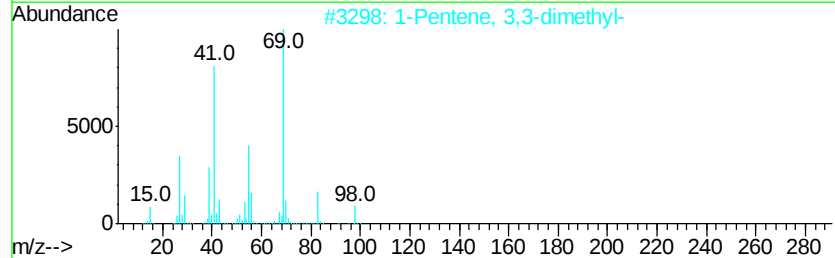
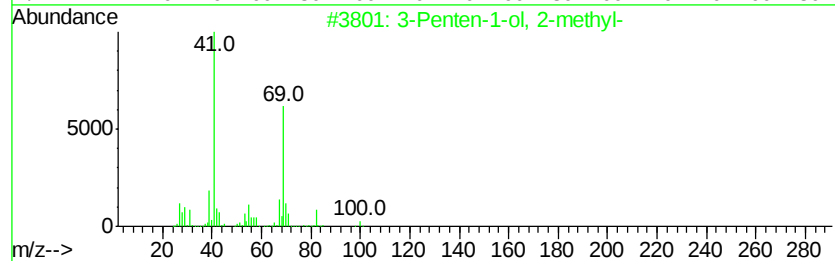
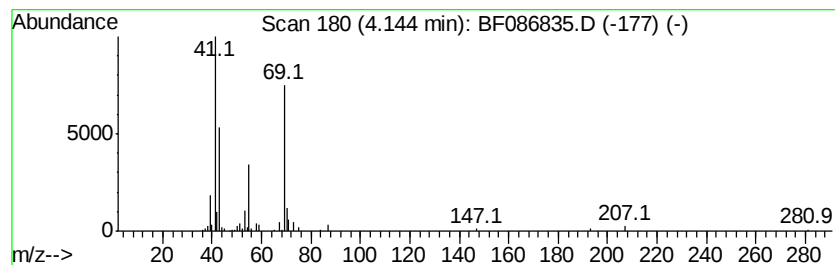
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-1-ol, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.14	6.15 ng	325247	1,4-Dichlorobenzene-d4	6.69

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-1-ol, 2-methyl-	100	C6H12O	062238-37-3	64
2			1-Pentene, 3,3-dimethyl-	98	C7H14	003404-73-7	45
3			1-Butene, 3,3-dimethyl-	84	C6H12	000558-37-2	40
4			1-Pentene, 3-ethyl-	98	C7H14	004038-04-4	39
5			1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	39



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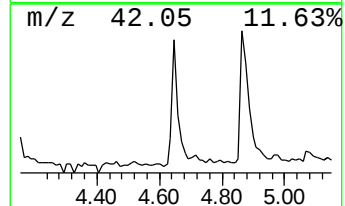
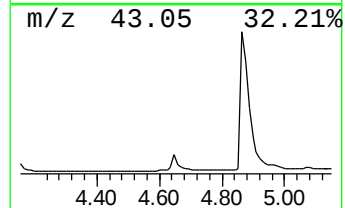
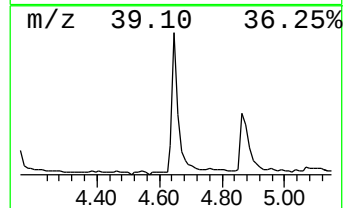
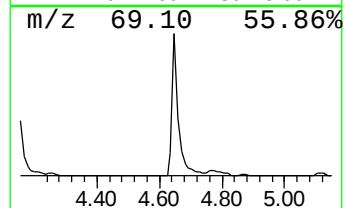
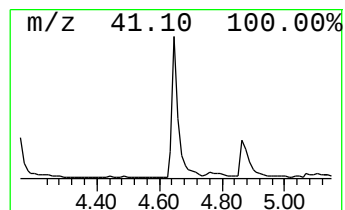
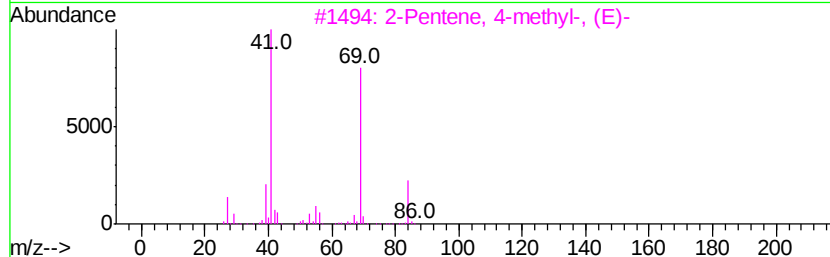
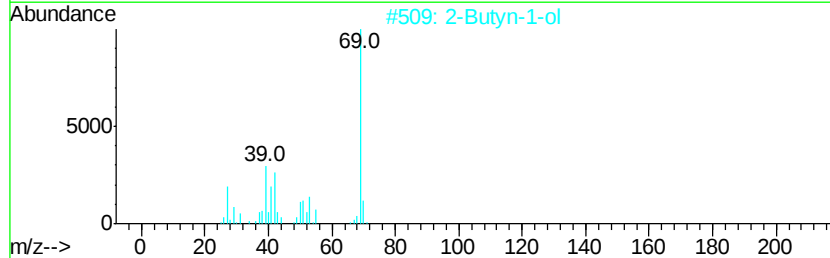
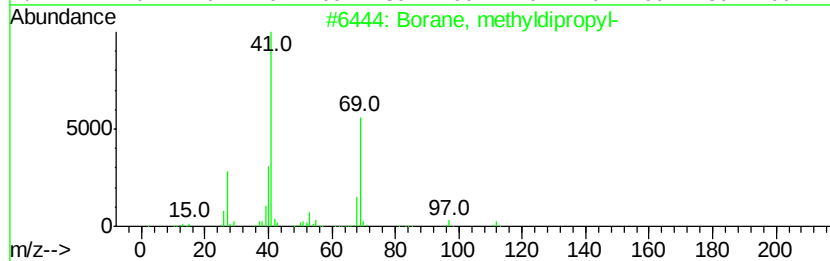
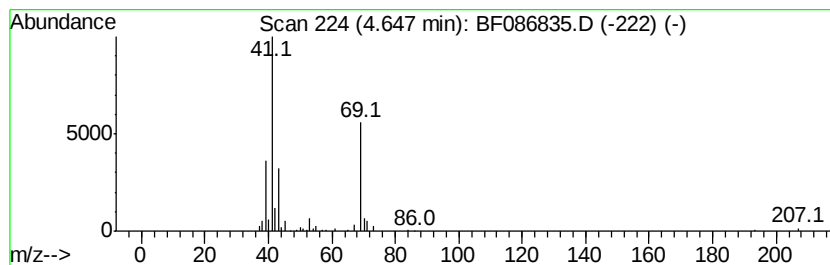
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown4.65 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.65	3.82 ng	201876	1,4-Dichlorobenzene-d4	6.69

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Borane, methylpropyl-	112	C7H17B	001117-21-1	36
2			2-Butyn-1-ol	70	C4H6O	000764-01-2	35
3			2-Pentene, 4-methyl-, (E)-	84	C6H12	000674-76-0	33
4			1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	28
5			Butane, 2,3-dimethyl-2-nitro-	131	C6H13NO2	034075-28-0	28



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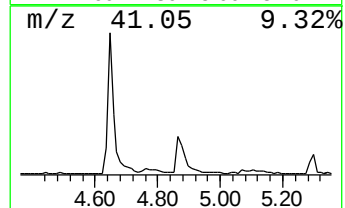
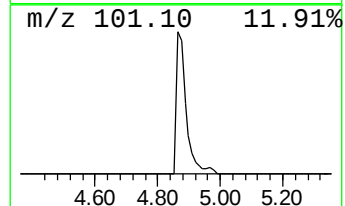
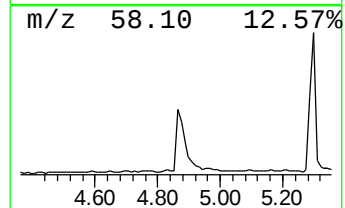
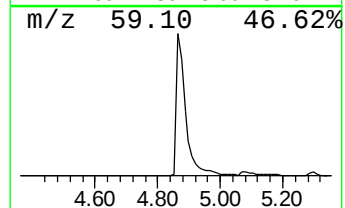
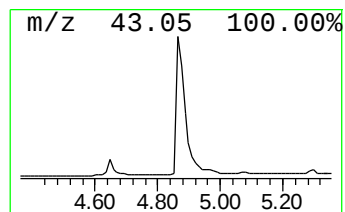
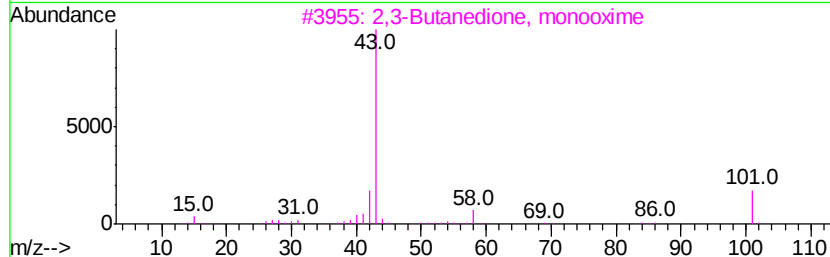
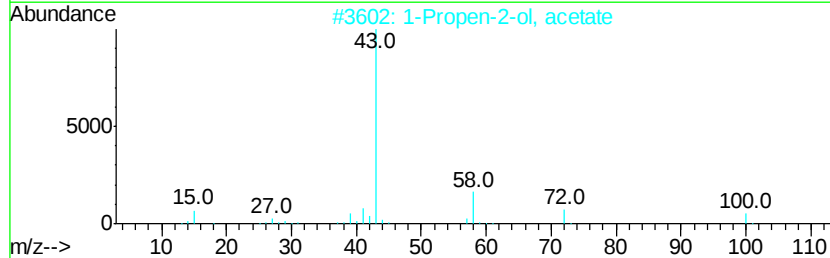
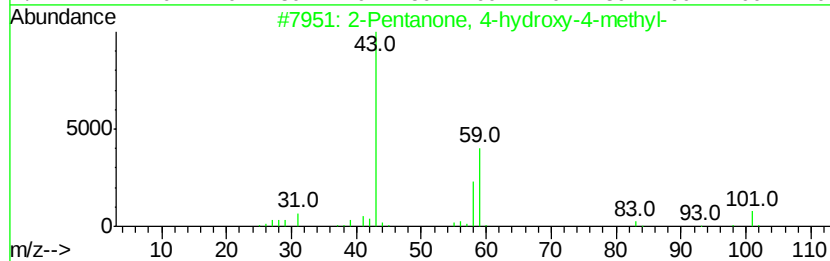
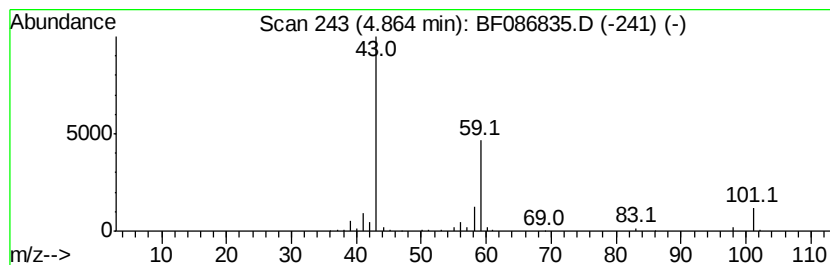
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	9.96 ng	527170	1,4-Dichlorobenzene-d4	6.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Diacetamide	101	C4H7NO2	000625-77-4	9
5		Butane	58	C4H10	000106-97-8	9



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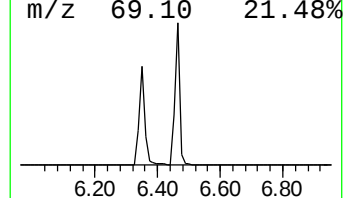
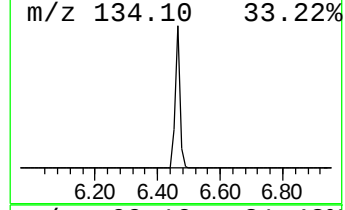
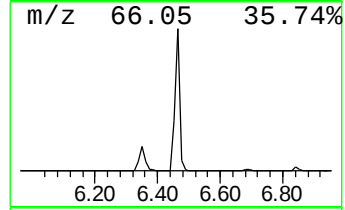
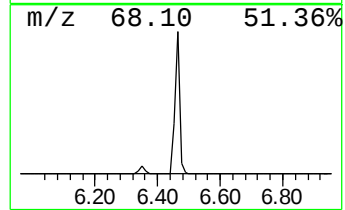
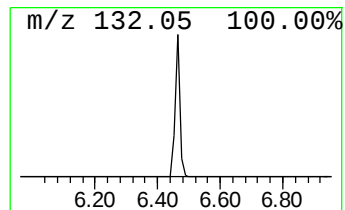
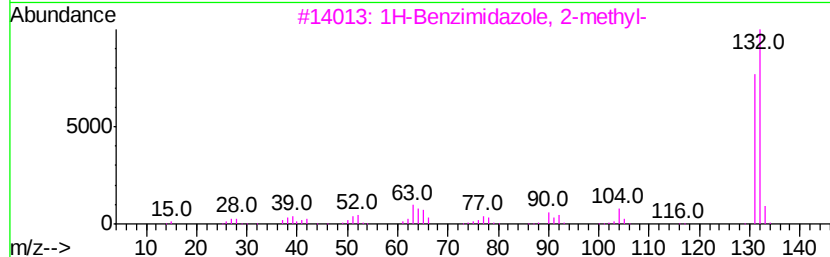
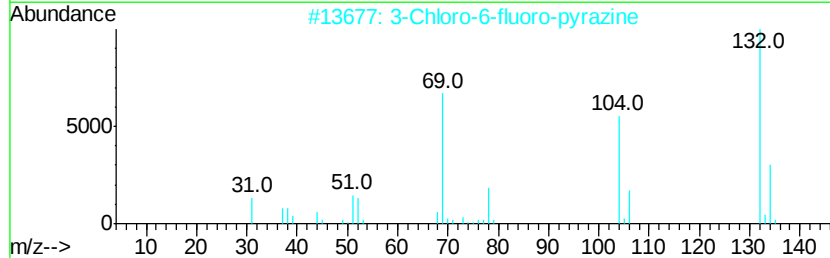
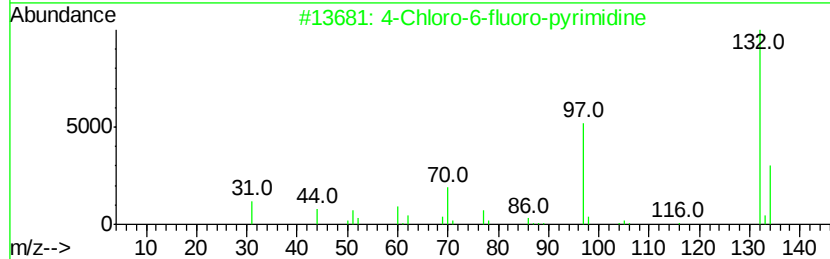
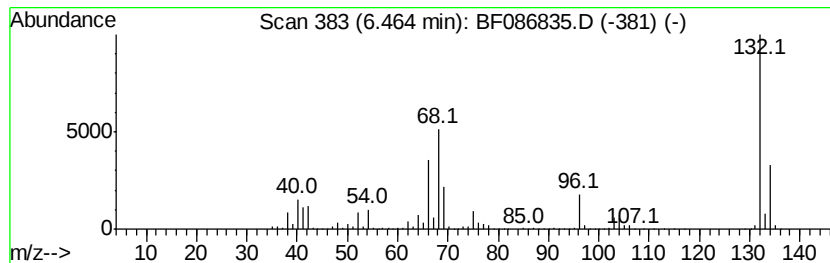
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	100.49 ng	5317230	1,4-Dichlorobenzene-d4	6.69

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



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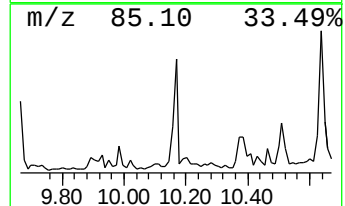
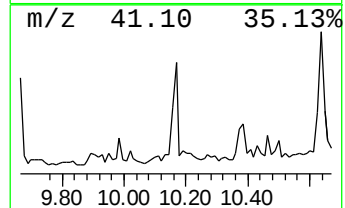
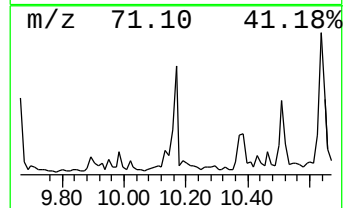
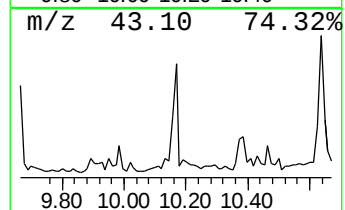
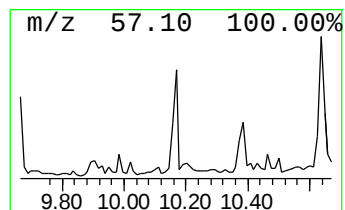
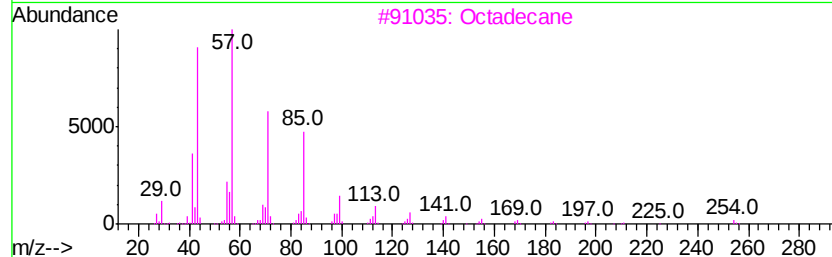
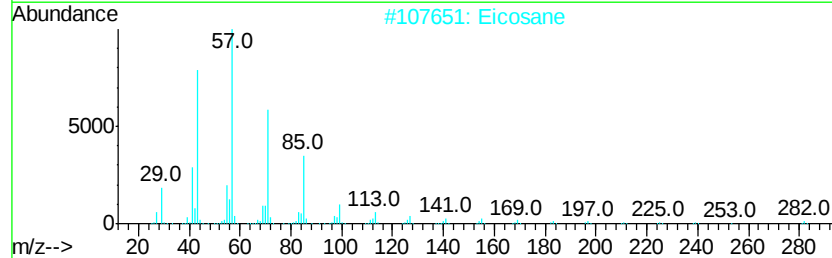
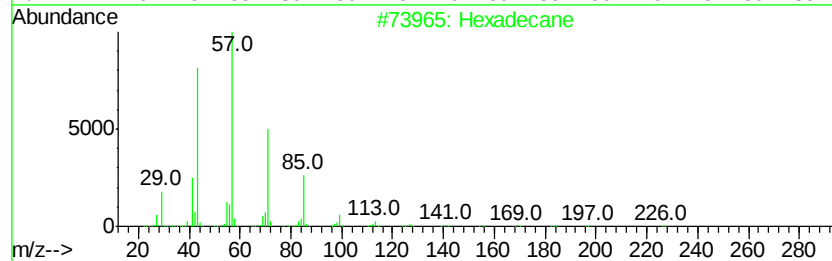
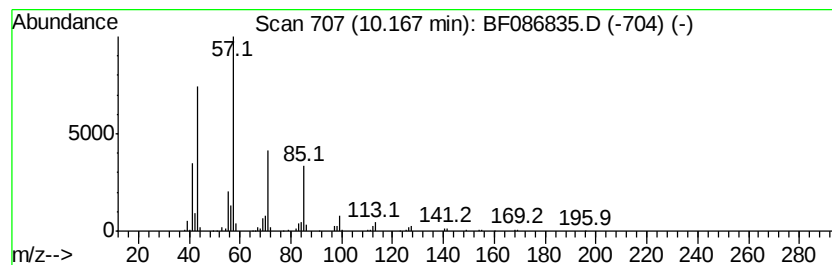
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.17	2.71 ng	216390	Acenaphthene-d10	9.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	90
2		Eicosane	282	C20H42	000112-95-8	90
3		Octadecane	254	C18H38	000593-45-3	80
4		Eicosane, 10-methyl-	296	C21H44	054833-23-7	72
5		Tetradecane	198	C14H30	000629-59-4	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050916\
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Acq On : 9 May 2016 22:05
Operator : UM/SJ
Sample : H2895-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

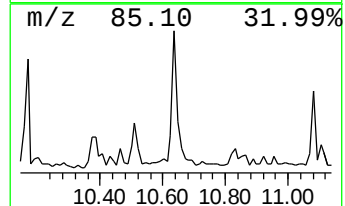
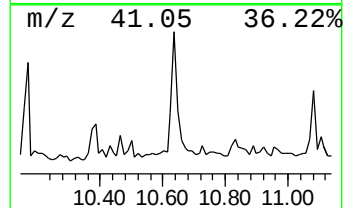
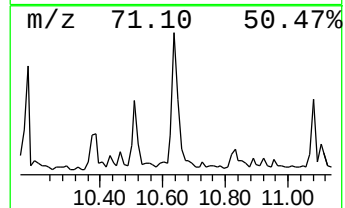
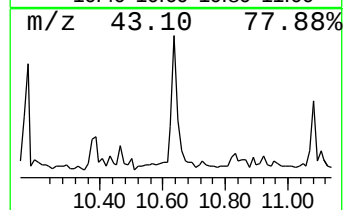
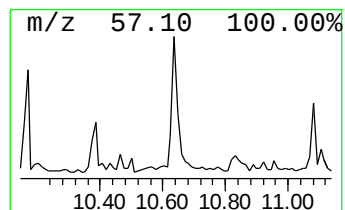
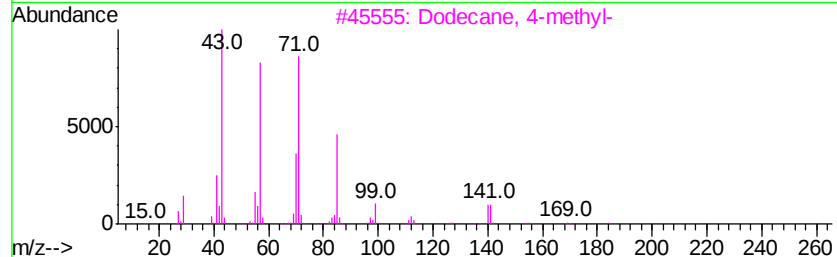
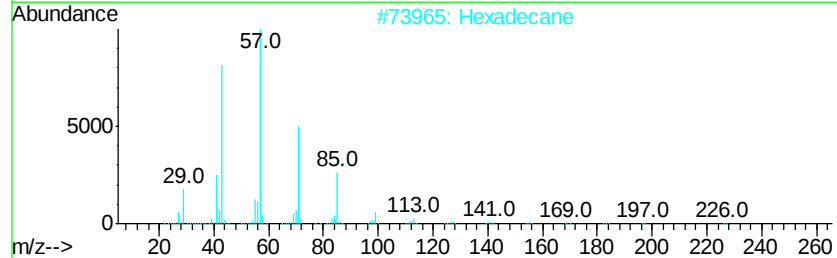
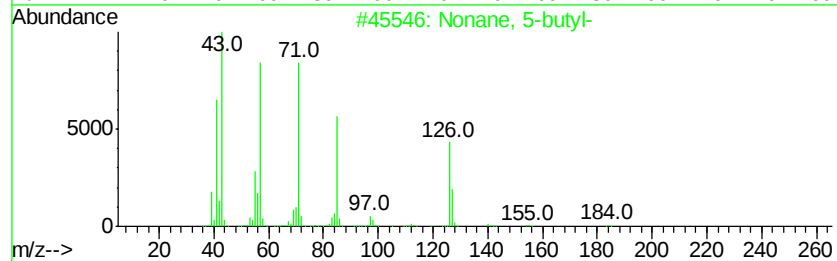
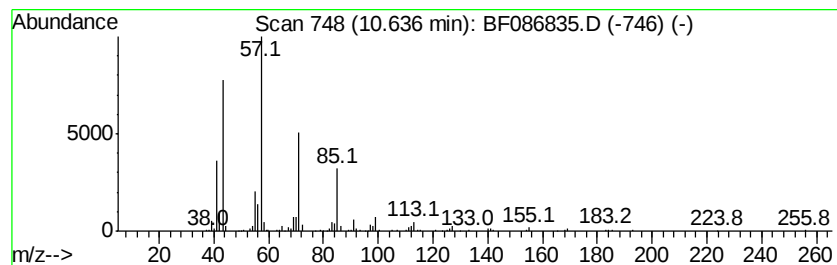
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonane, 5-butyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.64	4.14 ng	345973	Phenanthrene-d10		11.21
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 5-butyl-	184	C13H28	017312-63-9	91
2	Hexadecane	226	C16H34	000544-76-3	91
3	Dodecane, 4-methyl-	184	C13H28	006117-97-1	87
4	Eicosane	282	C20H42	000112-95-8	87
5	Tridecane, 7-propyl-	226	C16H34	055045-09-5	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050916\
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ClientSampleId :
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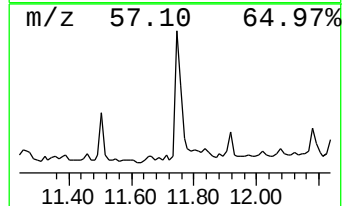
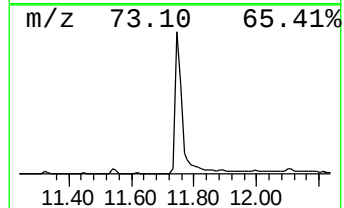
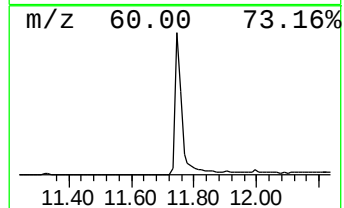
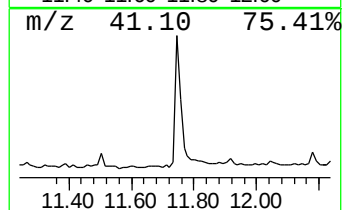
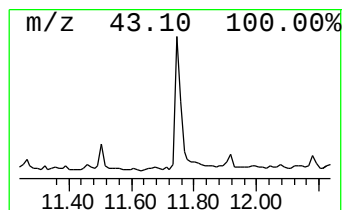
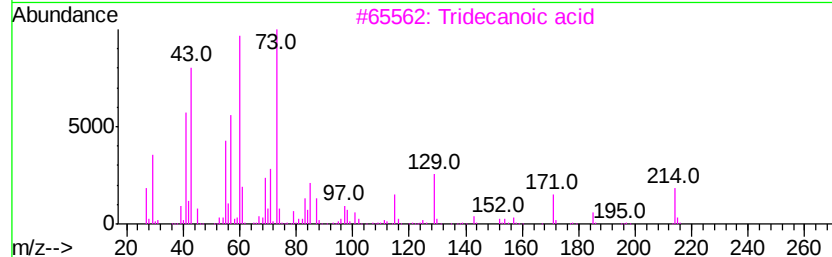
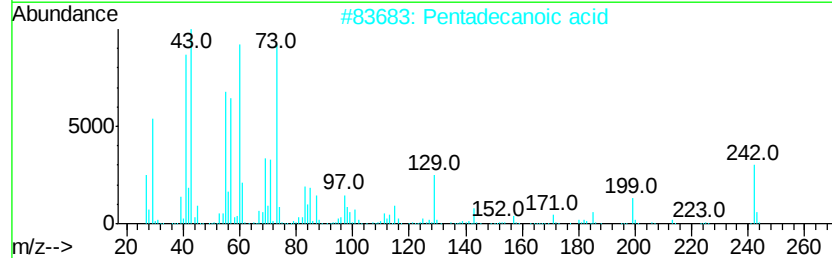
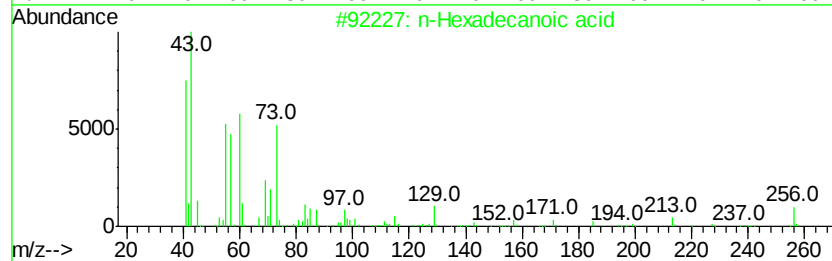
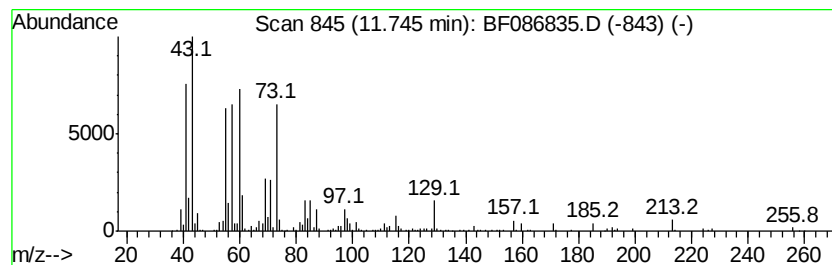
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.74	7.22 ng	602897	Phenanthrene-d10	11.21

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		Tridecanoic acid	214	C13H26O2	000638-53-9	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5		Undecanoic acid	186	C11H22O2	000112-37-8	78



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050916\
Data File : BF086835.D
Acq On : 9 May 2016 22:05
Operator : UM/SJ
Sample : H2895-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

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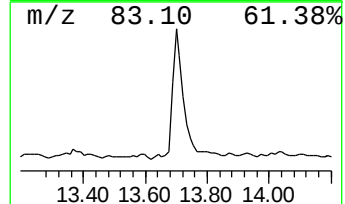
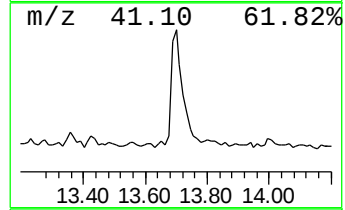
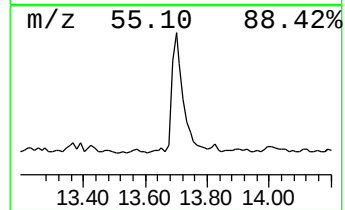
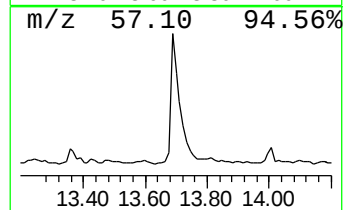
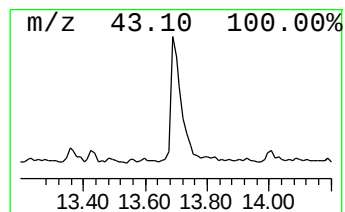
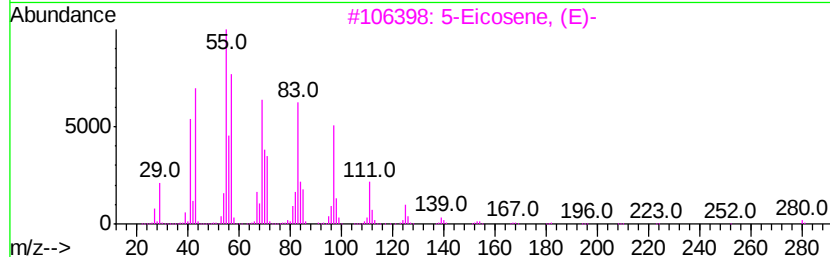
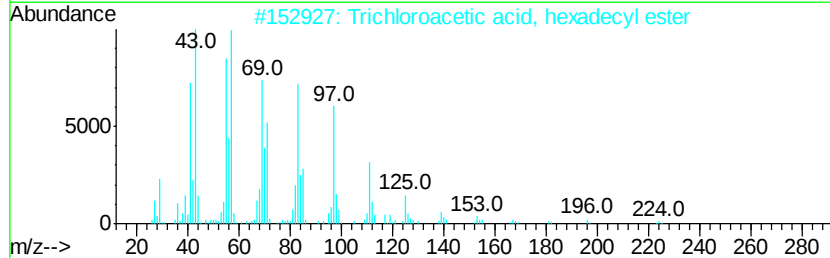
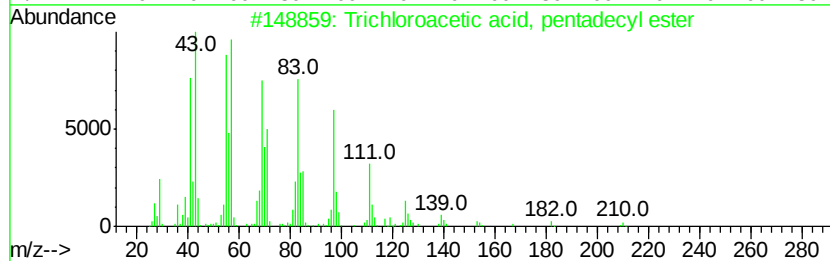
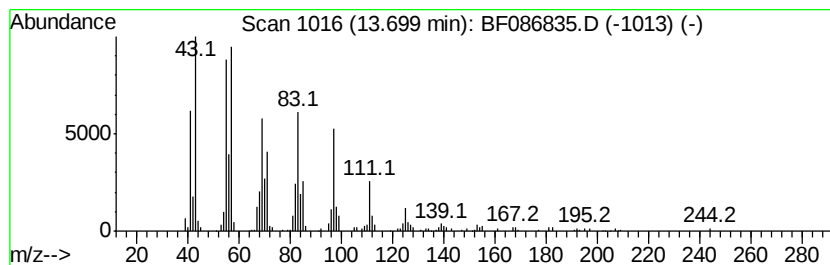
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Trichloroacetic acid, penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	7.59 ng	566005	Chrysene-d12	13.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3			5-Eicosene, (E)-	280	C20H40	074685-30-6	91
4			1-Docosene	308	C22H44	001599-67-3	91
5			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050916\
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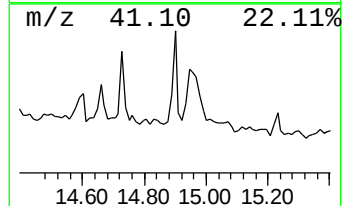
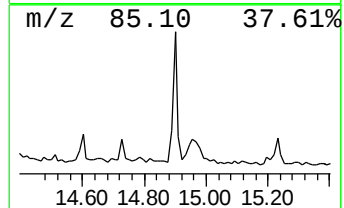
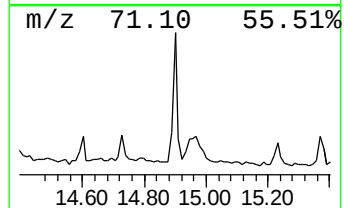
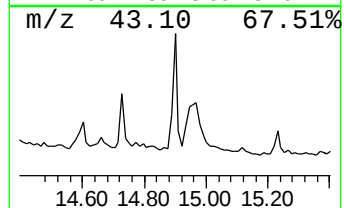
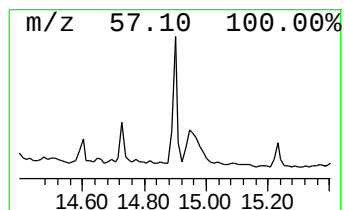
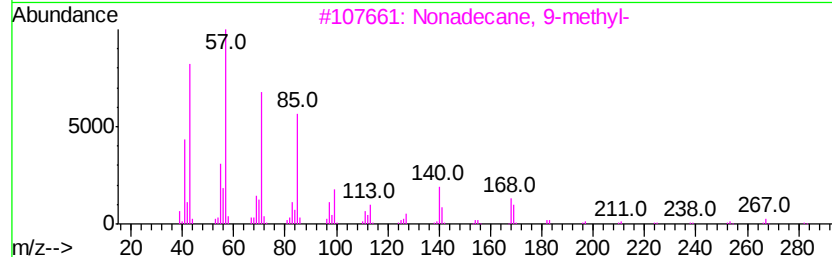
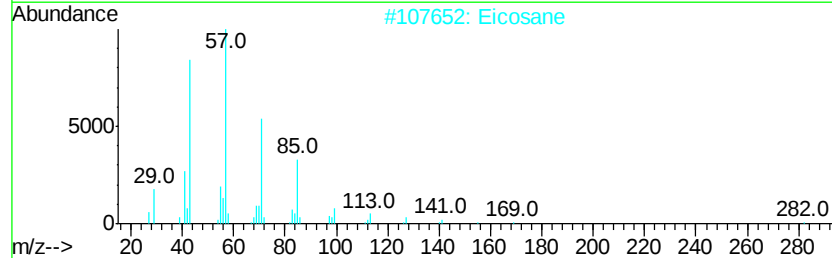
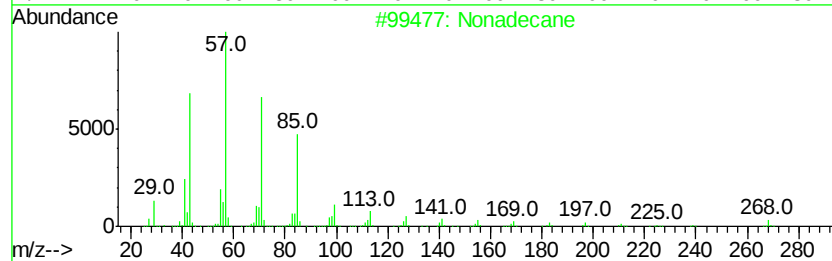
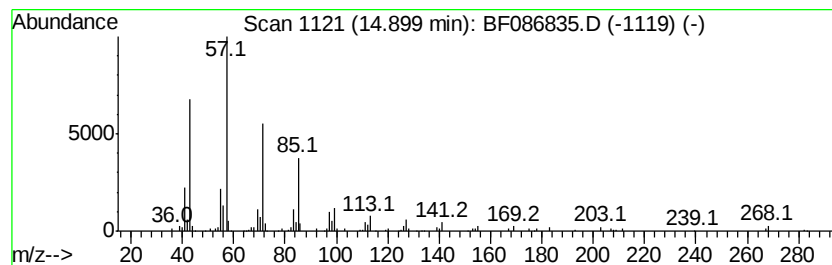
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Nonadecane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.90	2.21 ng	119224	Perylene-d12	15.21
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Nonadecane	268 C19H40	000629-92-5	97
2	Eicosane	282 C20H42	000112-95-8	96
3	Nonadecane, 9-methyl-	282 C20H42	013287-24-6	92
4	Hentriacontane	437 C31H64	000630-04-6	91
5	Tetratetracontane	619 C44H90	007098-22-8	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF050916\
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Misc :
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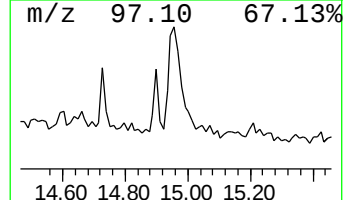
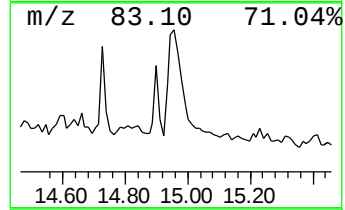
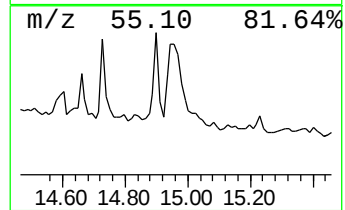
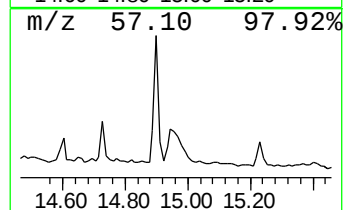
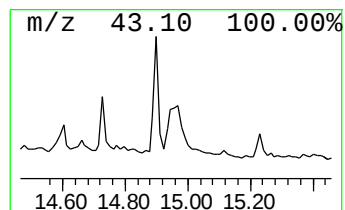
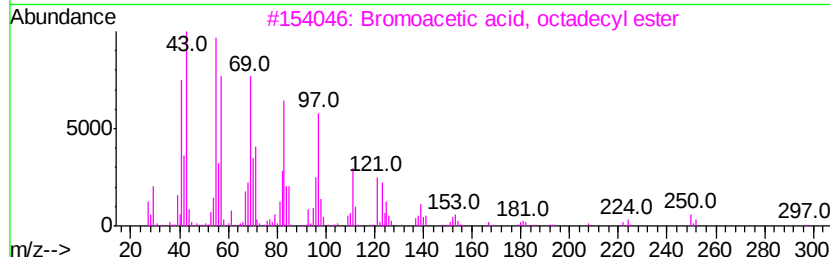
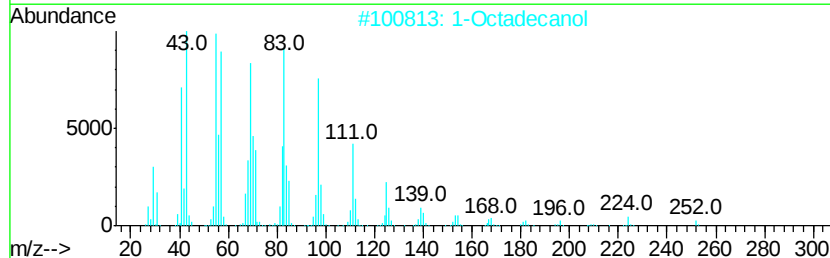
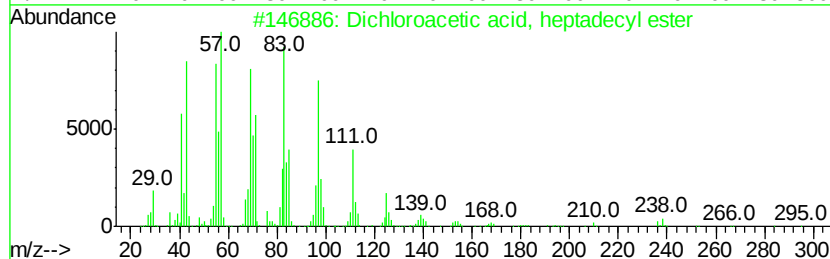
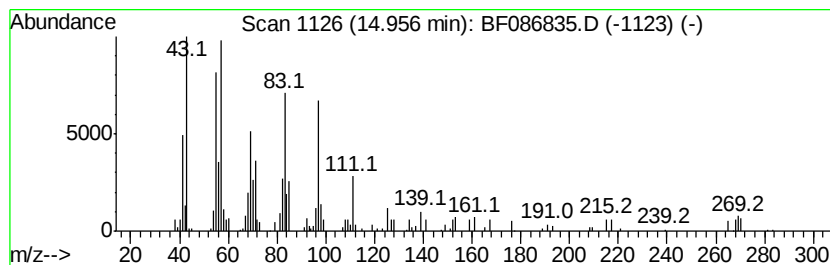
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Dichloroacetic acid, heptad... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	3.85 ng	207843	Perylene-d12	15.21

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87
2			1-Octadecanol	270	C18H38O	000112-92-5	83
3			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	80
4			2-Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	80
5			1-Nonadecanol	284	C19H40O	001454-84-8	74



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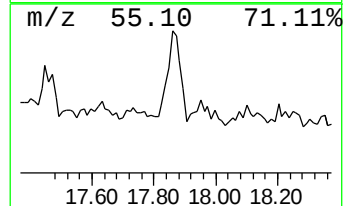
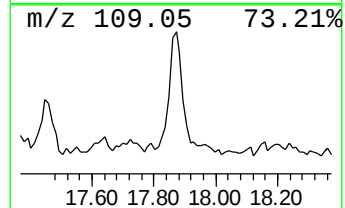
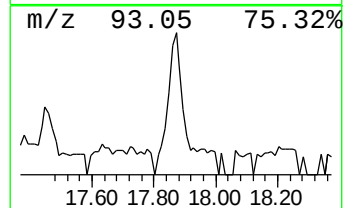
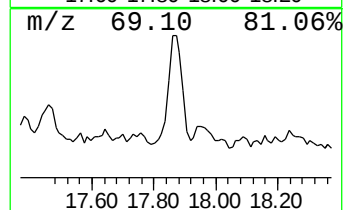
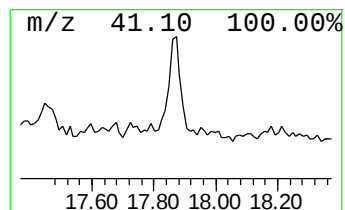
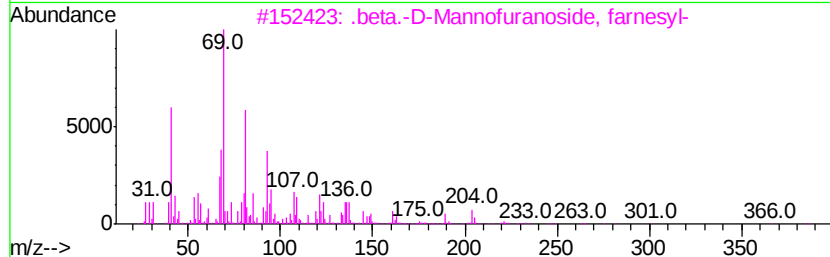
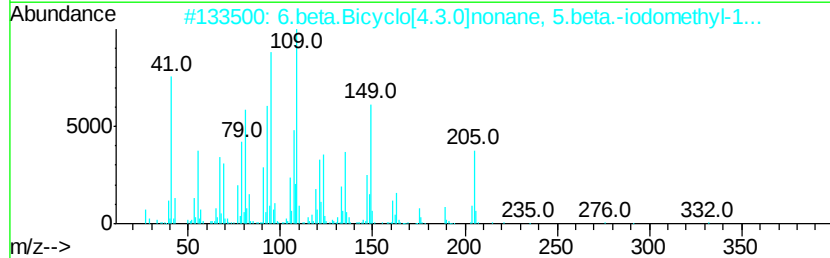
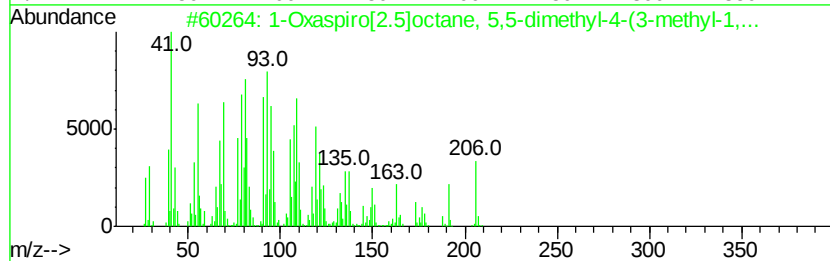
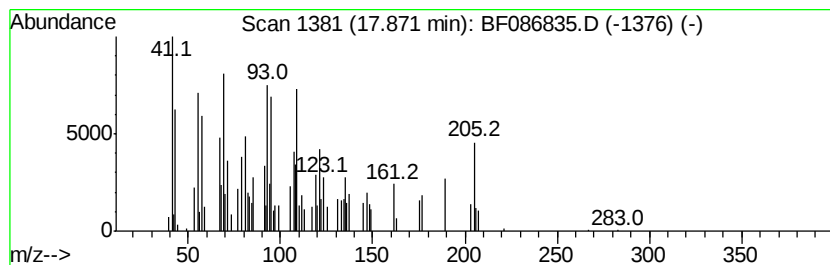
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown17.87 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.87	2.45 ng	132643	Perylene-d12	15.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Oxaspiro[2.5]octane, 5,5-dimet...	206	C14H22O	1000195-92-1	49
2		6.beta.Bicyclo[4.3.0]nonane, 5.b...	332	C15H25I	1000195-85-9	49
3		.beta.-D-Mannofuranoside, farnesyl-	384	C21H36O6	1000155-15-5	27
4		1,6,10-Dodecatriene, 7,11-dimeth...	204	C15H24	018794-84-8	27
5		2,6,10,14-Hexadecatetraen-1-ol, ...	332	C22H36O2	061691-98-3	27



Data Path : Z:\HPCHEM1\BNA F\DATA\BF050916\
Data File : BF086835.D
Acq On : 9 May 2016 22:05
Operator : UM/SJ
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Misc :
ALS Vial : 9 Sample Multiplier: 1

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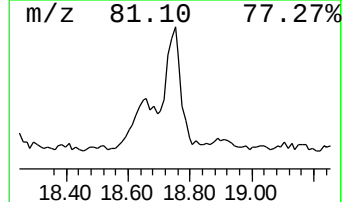
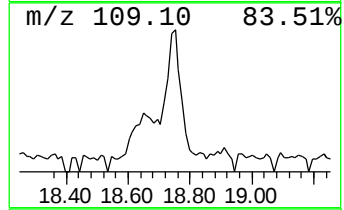
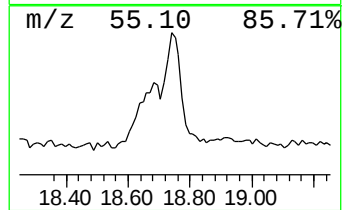
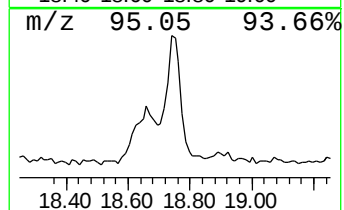
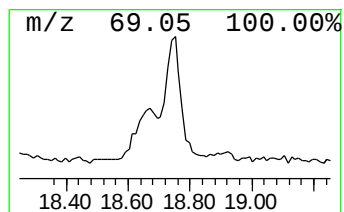
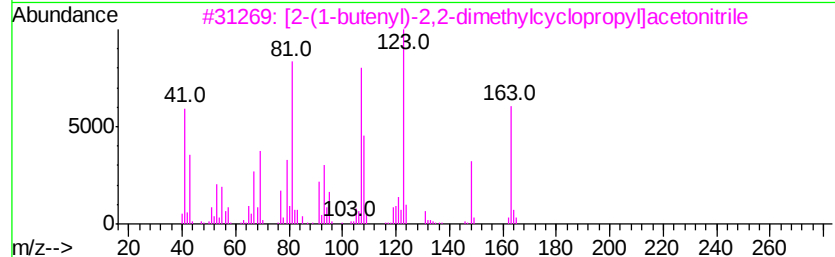
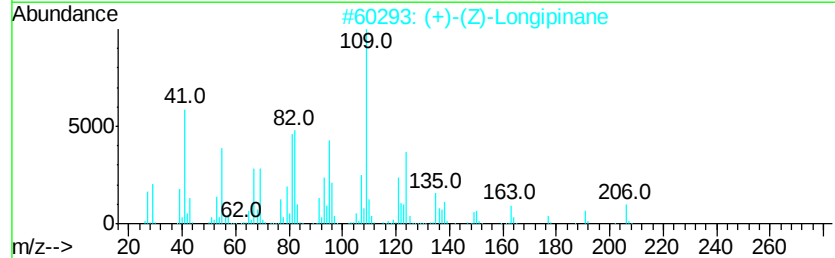
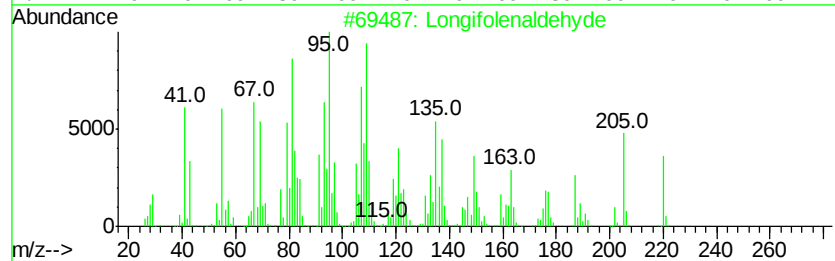
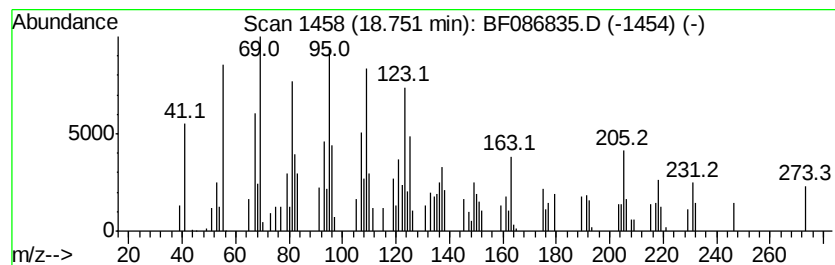
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Longifolenaldehyde Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.75	4.99 ng	269834	Perylene-d12	15.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Longifolenaldehyde	220	C15H24O	019890-84-7	53
2		(+)-(Z)-Longipinane	206	C15H26	1000156-12-3	47
3		[2-(1-butenyl)-2,2-dimethylcyclopropyl]acetonitrile	163	C11H17N	1000111-15-4	41
4		Cyclohexanone, 2,3,3-trimethyl-2-methylene-	206	C14H22O	069296-90-8	38
5		13-Tetradecene-11-yn-1-ol	208	C14H24O	1000131-00-4	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050916\
 Data File : BF086835.D
 Acq On : 9 May 2016 22:05
 Operator : UM/SJ
 Sample : H2895-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP1-6-9FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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
3-Penten-1-ol, 2-...	4.14	6.2	ng	325247	1	6.69	1058230	20.0
unknown4.65	4.65	3.8	ng	201876	1	6.69	1058230	20.0
2-Pentanone, 4-hy...	4.86	10.0	ng	527170	1	6.69	1058230	20.0
unknown6.46	6.46	100.5	ng	5317230	1	6.69	1058230	20.0
Hexadecane	10.17	2.7	ng	216390	3	9.72	1598910	20.0
Nonane, 5-butyl-	10.64	4.1	ng	345973	4	11.21	1670680	20.0
n-Hexadecanoic acid	11.74	7.2	ng	602897	4	11.21	1670680	20.0
Trichloroacetic a...	13.70	7.6	ng	566005	5	13.82	1490770	20.0
Nonadecane	14.90	2.2	ng	119224	6	15.21	1080910	20.0
Dichloroacetic ac...	14.96	3.9	ng	207843	6	15.21	1080910	20.0
unknown17.87	17.87	2.5	ng	132643	6	15.21	1080910	20.0
Longifolenaldehyde	18.75	5.0	ng	269834	6	15.21	1080910	20.0