

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082015\
 Data File : BF081136.D
 Acq On : 20 Aug 2015 21:13
 Operator : UM/IZ
 Sample : G3282-07
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB04-4.0-5.0-081115

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-BF081715.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	3.956	178	181	186	rBV	55463	96413	4.01%	0.433%
2	4.710	243	247	256	rBV	1195223	2162106	90.03%	9.713%
3	5.156	283	286	288	rBV	1954424	2127007	88.57%	9.555%
4	5.567	320	322	325	rVB	92184	80385	3.35%	0.361%
5	6.230	376	380	382	rBV	2052431	2401598	100.00%	10.789%
6	6.344	387	390	392	rBV	2243755	2303451	95.91%	10.348%
7	6.573	408	410	412	rBV	579136	476360	19.84%	2.140%
8	6.733	421	424	426	rBV	1703873	1625999	67.70%	7.305%
9	7.144	457	460	463	rBV	1347714	1418306	59.06%	6.372%
10	7.784	514	516	520	rBV	42349	43993	1.83%	0.198%
11	7.864	520	523	525	rVB	558796	621029	25.86%	2.790%
12	7.956	529	531	533	rBV	17168	25631	1.07%	0.115%
13	8.939	614	617	620	rBV	1647145	1932102	80.45%	8.680%
14	9.339	650	652	654	rBV	423613	355727	14.81%	1.598%
15	9.385	654	656	660	rVV	75821	99203	4.13%	0.446%
16	9.602	673	675	678	rVB	498633	655313	27.29%	2.944%
17	10.059	714	715	717	rVB	33250	24836	1.03%	0.112%
18	10.390	741	744	747	rVB	1236936	1177543	49.03%	5.290%
19	10.528	755	756	761	rVB	52421	60368	2.51%	0.271%
20	10.733	771	774	777	rBV	31792	45872	1.91%	0.206%
21	10.848	780	784	787	rBV3	14939	30311	1.26%	0.136%
22	10.973	793	795	796	rBV	49643	39632	1.65%	0.178%
23	11.076	802	804	806	rVB	766357	657262	27.37%	2.953%
24	11.396	830	832	835	rBV	26159	25191	1.05%	0.113%
25	11.636	850	853	856	rBV2	19556	46930	1.95%	0.211%
26	11.888	872	875	877	rBV4	14417	27744	1.16%	0.125%
27	12.505	927	929	933	rBV	170783	164216	6.84%	0.738%
28	12.585	933	936	937	rBV2	48439	69760	2.90%	0.313%
29	12.665	940	943	945	rBV	1958114	1907269	79.42%	8.568%
30	12.951	966	968	971	rBV2	27995	60802	2.53%	0.273%
31	13.214	988	991	992	rBV	101934	125194	5.21%	0.562%
32	13.259	992	995	998	rVV	66926	114738	4.78%	0.515%
33	13.579	1019	1023	1026	rBV3	90397	217794	9.07%	0.978%
34	13.694	1030	1033	1035	rBV	570271	544791	22.68%	2.447%

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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-BF081715.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.899	1049	1051	1053	rBV	67702	76032	3.17%	0.342%
36	14.471	1099	1101	1102	rBV	58892	79771	3.32%	0.358%
37	15.031	1148	1150	1153	rVB	241791	339118	14.12%	1.523%

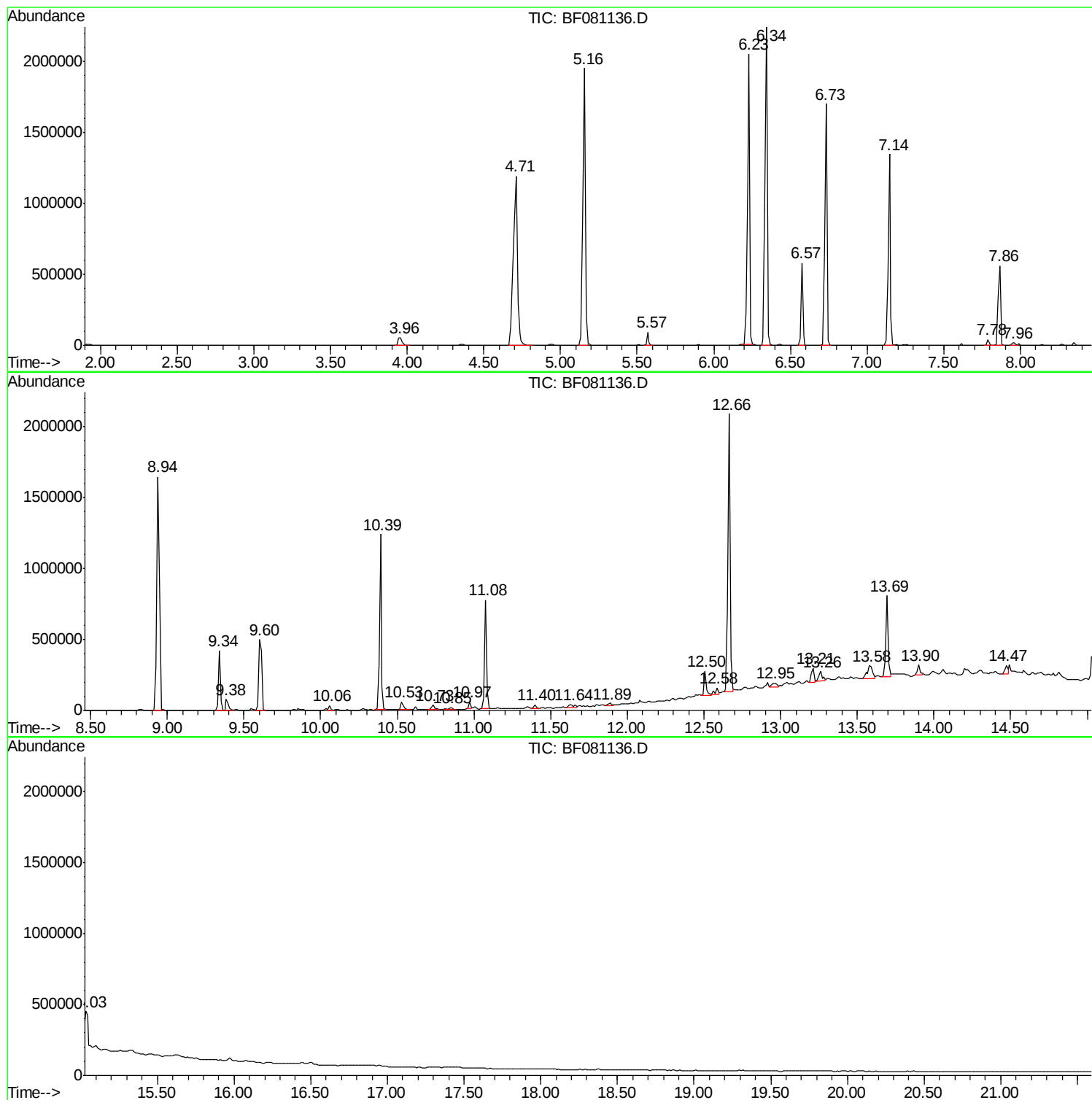
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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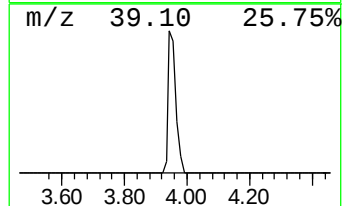
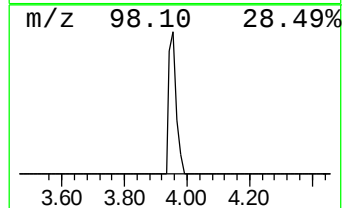
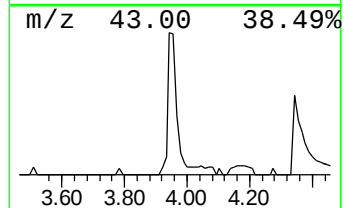
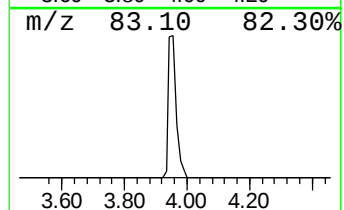
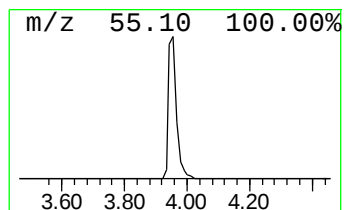
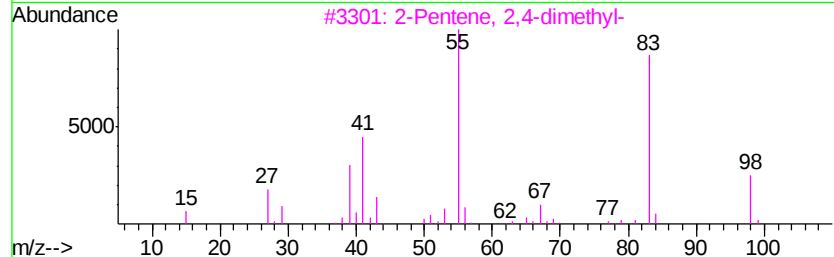
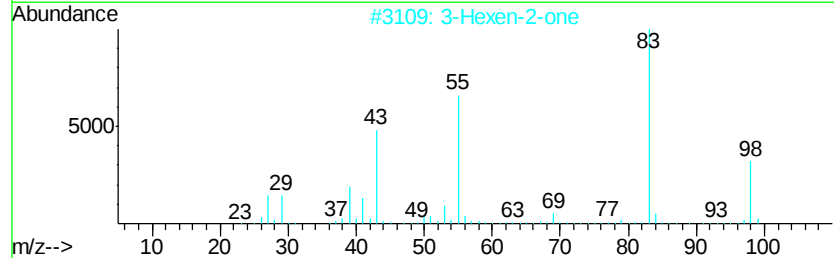
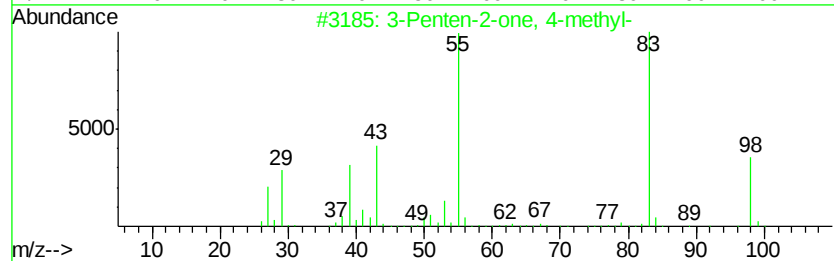
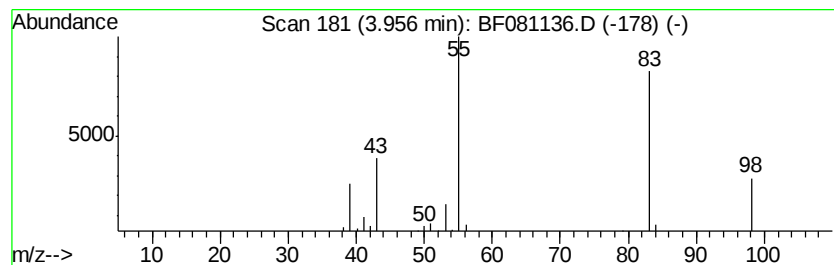
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.96	4.05 ng	96413	1,4-Dichlorobenzene-d4	6.57

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	86
3			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80
5			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	80



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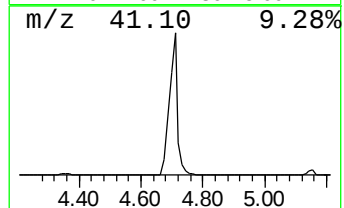
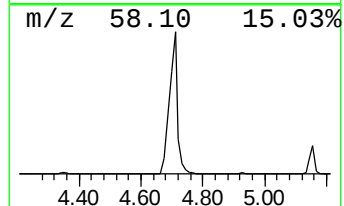
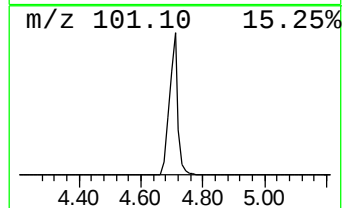
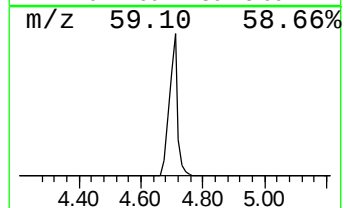
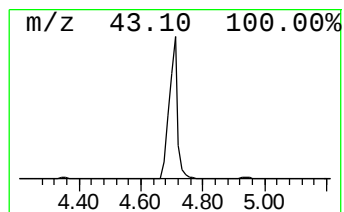
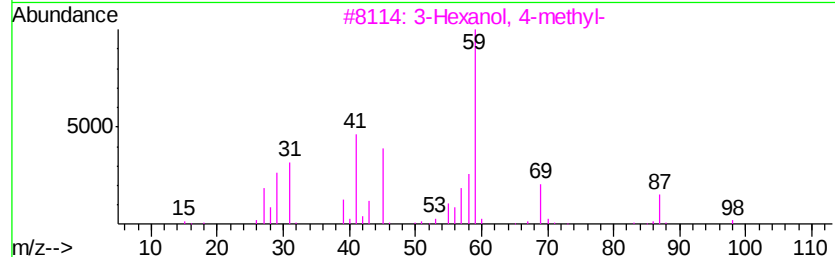
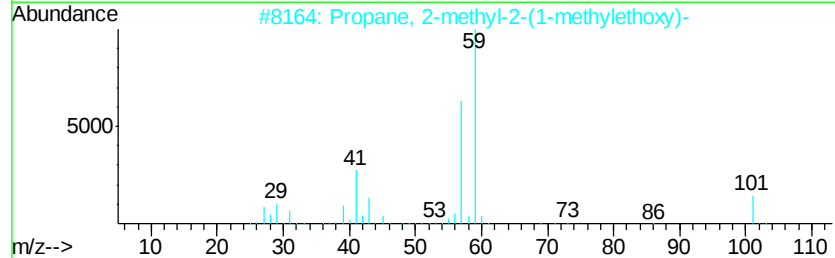
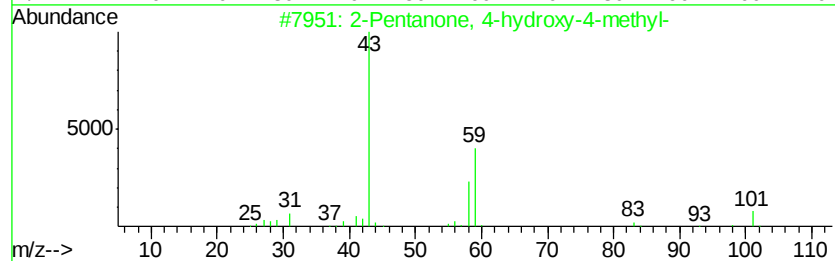
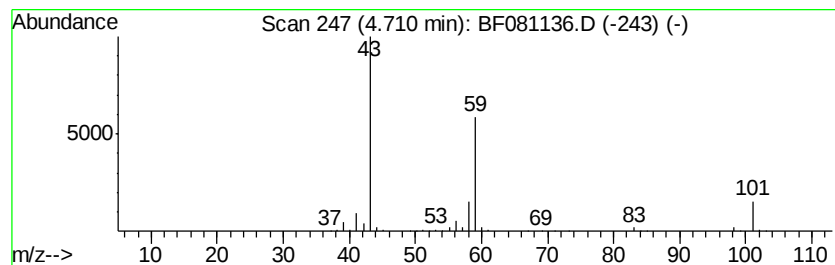
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.71	90.78 ng	2162110	1,4-Dichlorobenzene-d4	6.57

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32



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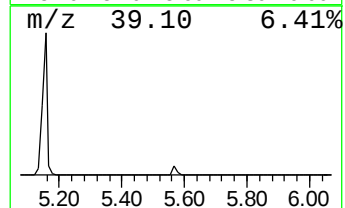
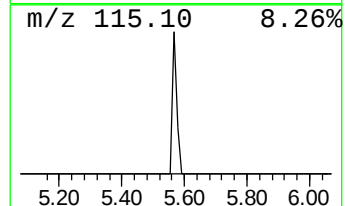
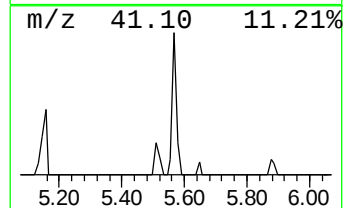
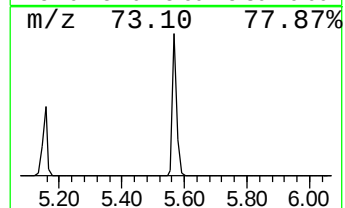
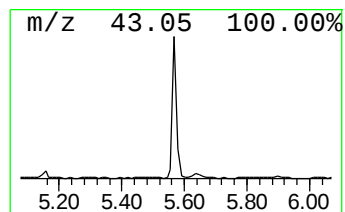
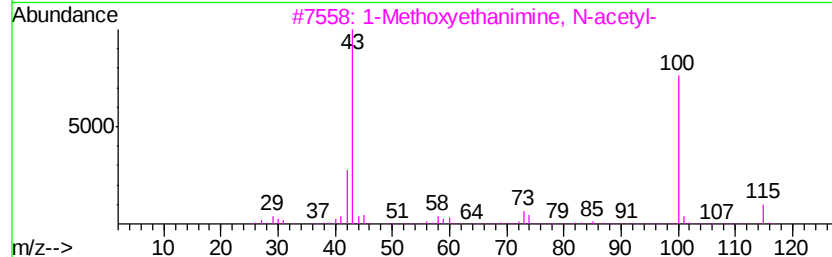
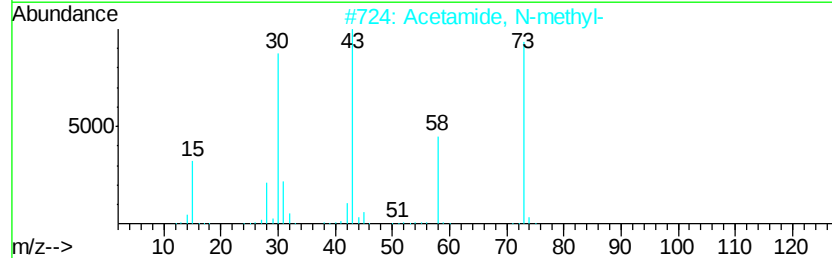
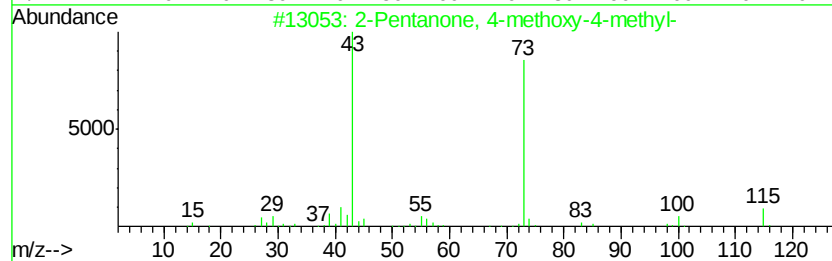
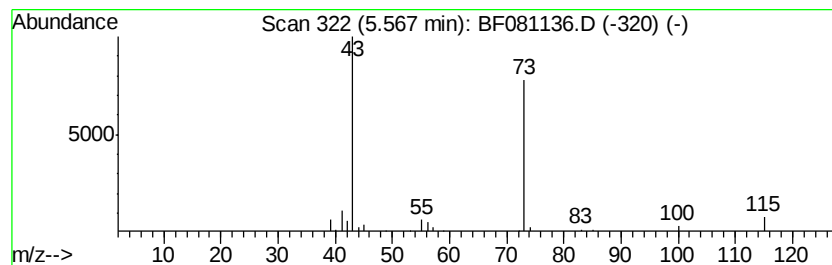
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.57	3.37 ng	80385	1,4-Dichlorobenzene-d4	6.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	90
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
3		1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	12
4		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	12
5		Hexane, 2-methyl-	100	C7H16	000591-76-4	9



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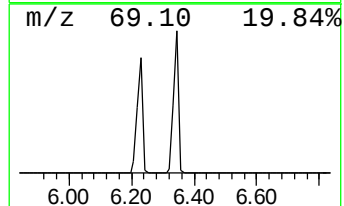
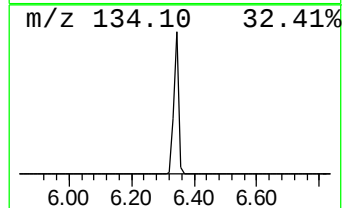
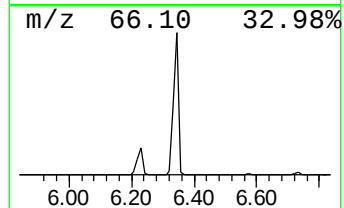
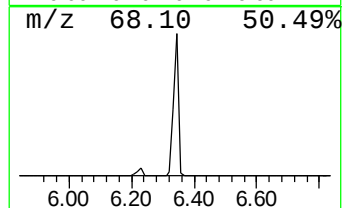
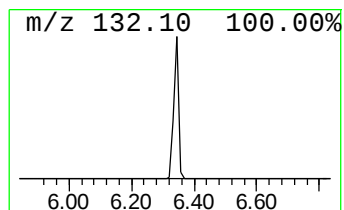
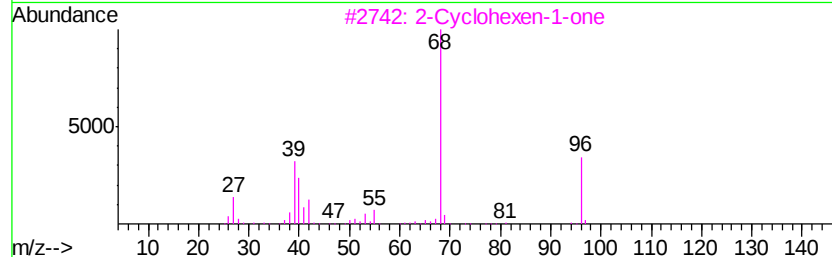
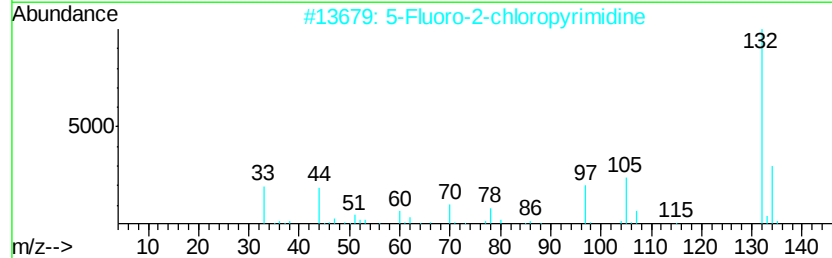
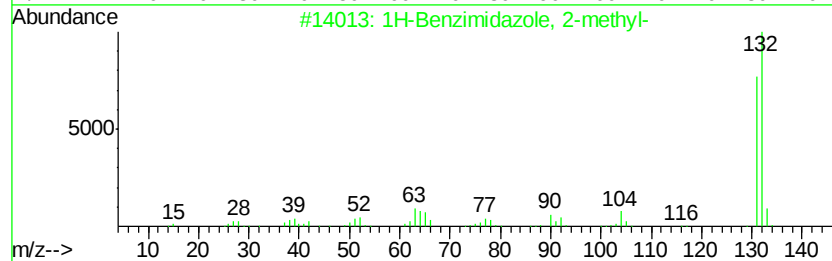
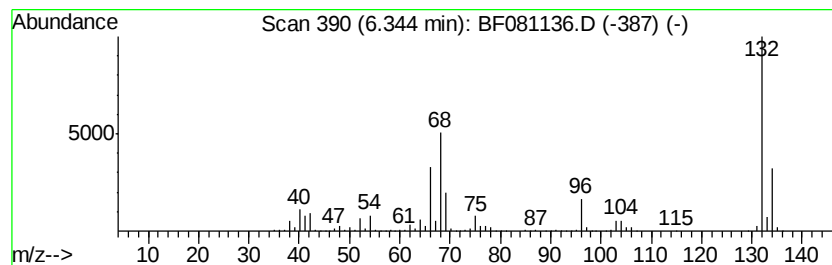
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.34 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	96.71 ng	2303450	1,4-Dichlorobenzene-d4	6.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	25
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
4		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5		1,1-Difluoro-3-methyl-1-silacycl...	134	C5H8F2Si	054077-66-6	9



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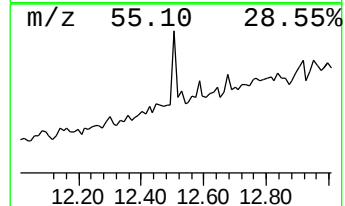
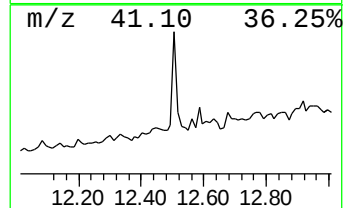
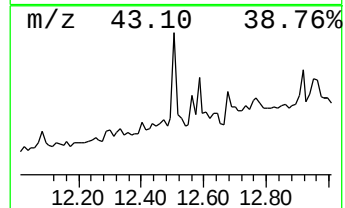
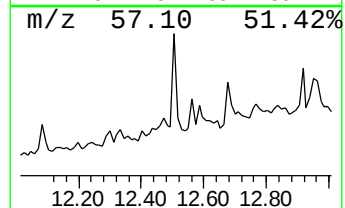
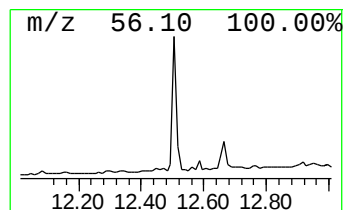
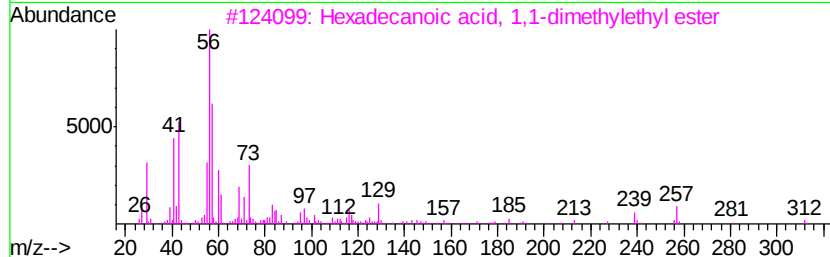
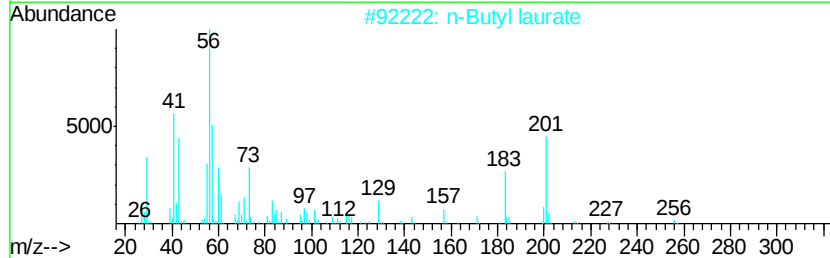
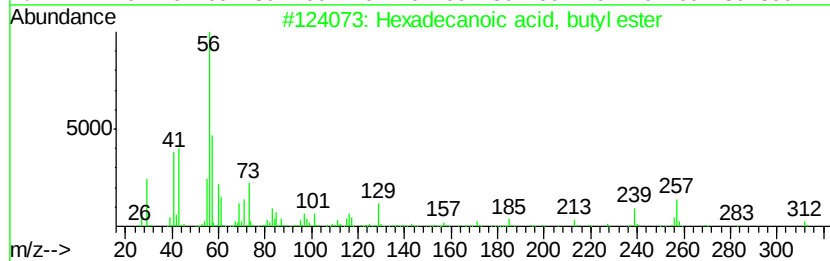
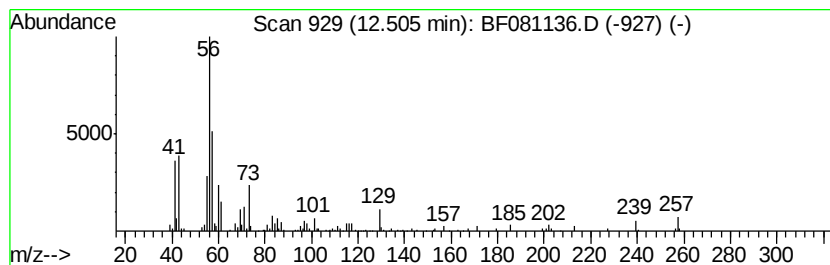
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.51	6.03 ng	164216	Chrysene-d12	13.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		n-Butyl laurate	256	C16H32O2	000106-18-3	83
3		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	49
4		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	46
5		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082015\
Data File : BF081136.D
Acq On : 20 Aug 2015 21:13
Operator : UM/IZ
Sample : G3282-07
Misc :
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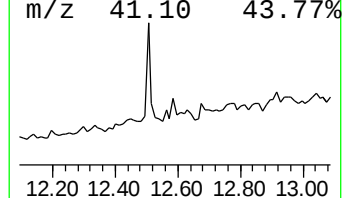
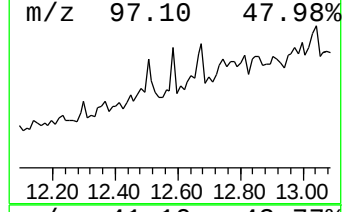
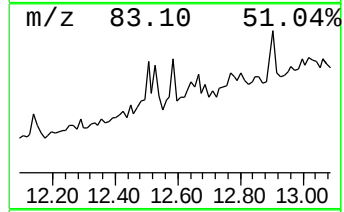
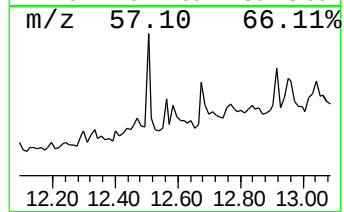
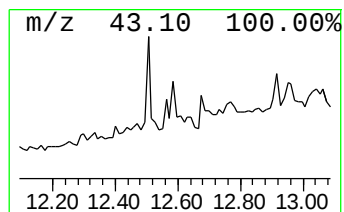
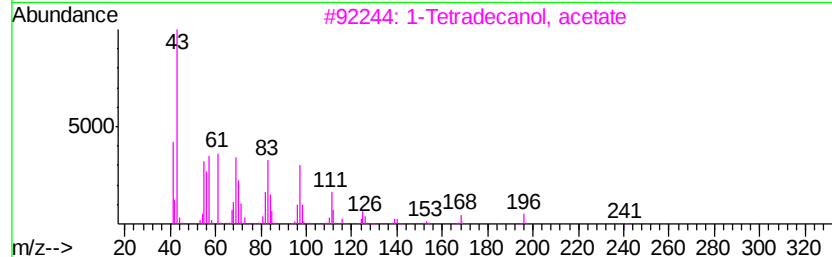
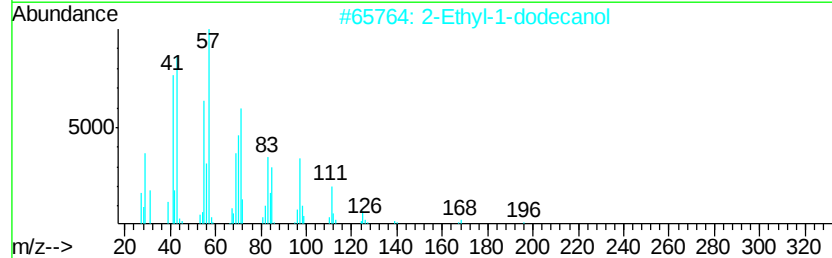
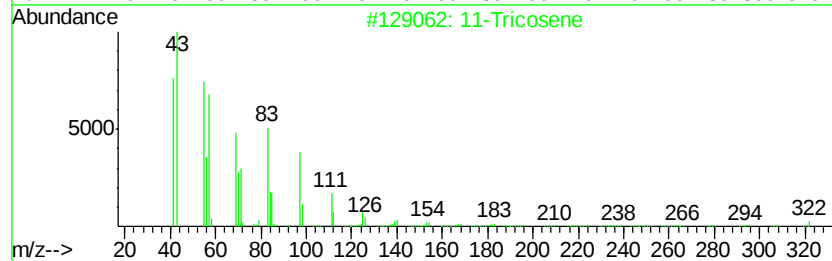
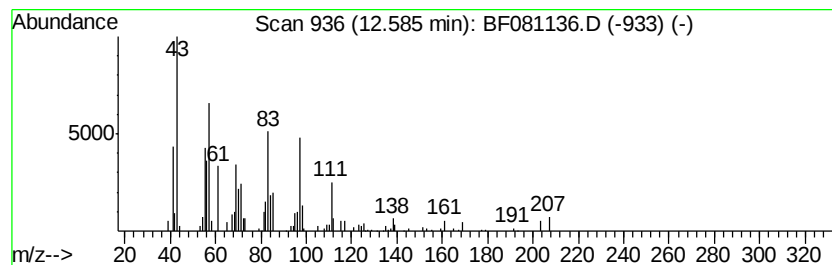
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 11-Tricosene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.59	2.56 ng	69760	Chrysene-d12	13.69
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	11-Tricosene	322 C23H46	052078-56-5	53
2	2-Ethyl-1-dodecanol	214 C14H30O	019780-33-7	50
3	1-Tetradecanol, acetate	256 C16H32O2	000638-59-5	46
4	1-Octadecene	252 C18H36	000112-88-9	43
5	Acetic acid, octadecyl ester	312 C20H40O2	000822-23-1	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082015\
Data File : BF081136.D
Acq On : 20 Aug 2015 21:13
Operator : UM/IZ
Sample : G3282-07
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ClientSampleId :
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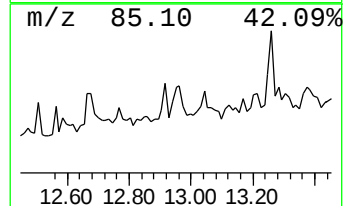
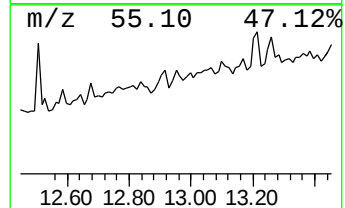
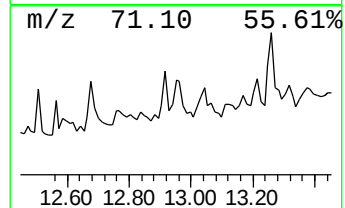
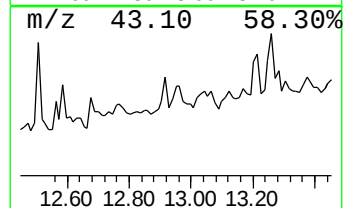
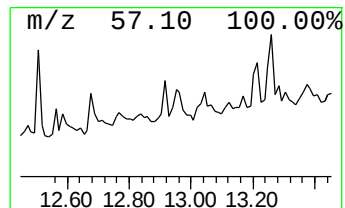
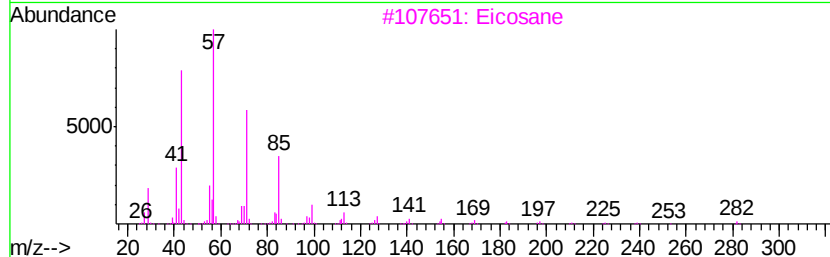
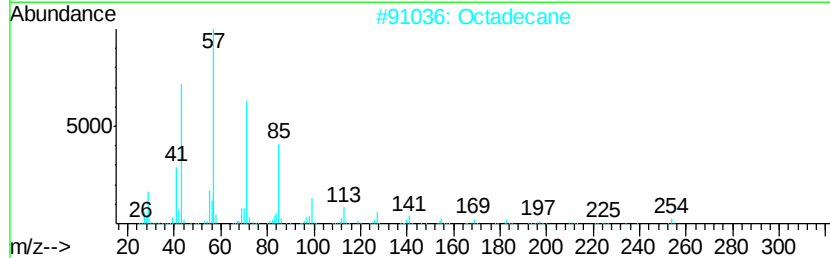
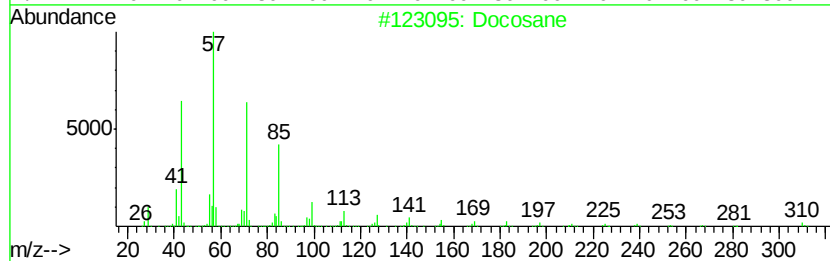
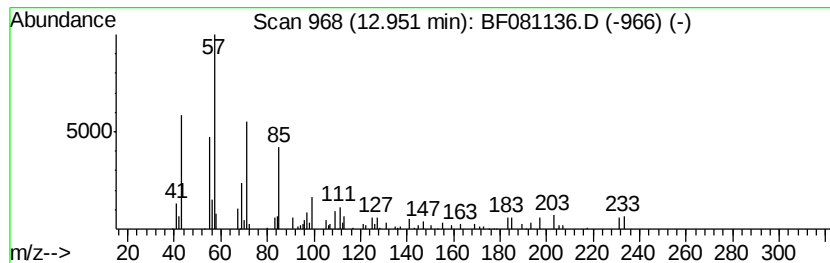
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Docosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.95	2.23 ng	60802	Chrysene-d12	13.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane	310	C22H46	000629-97-0	64
2		Octadecane	254	C18H38	000593-45-3	64
3		Eicosane	282	C20H42	000112-95-8	59
4		Heneicosane	296	C21H44	000629-94-7	59
5		Tetratetracontane	619	C44H90	007098-22-8	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082015\
Data File : BF081136.D
Acq On : 20 Aug 2015 21:13
Operator : UM/IZ
Sample : G3282-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

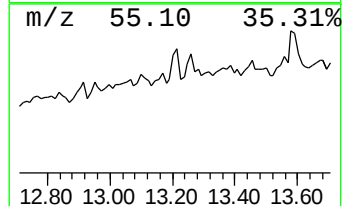
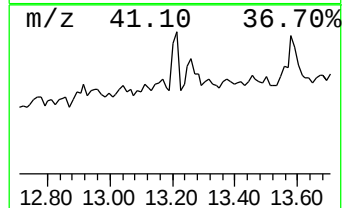
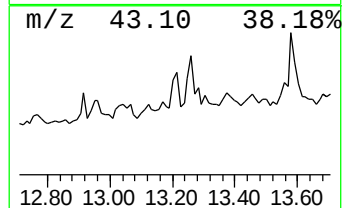
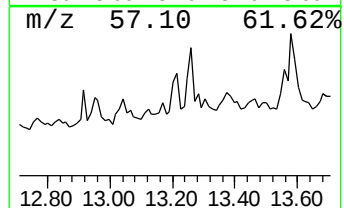
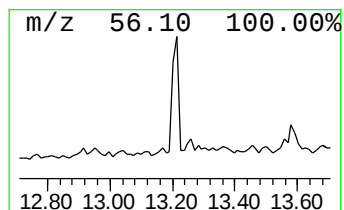
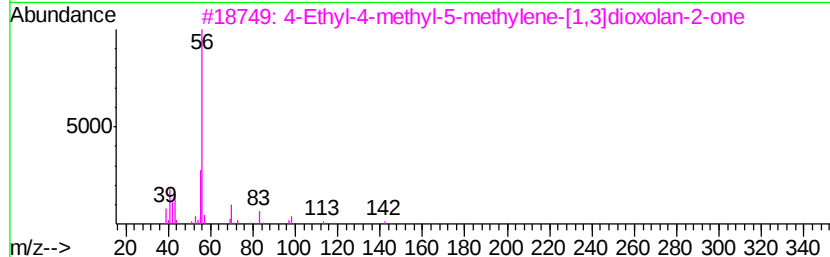
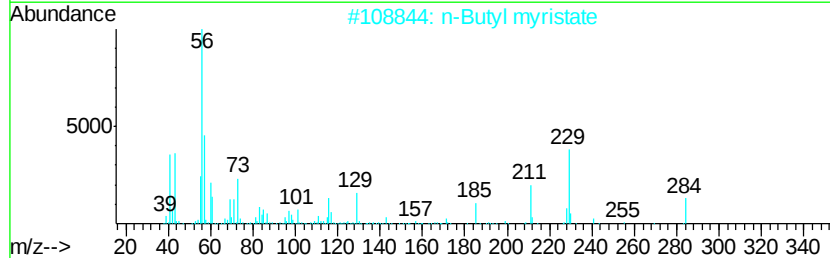
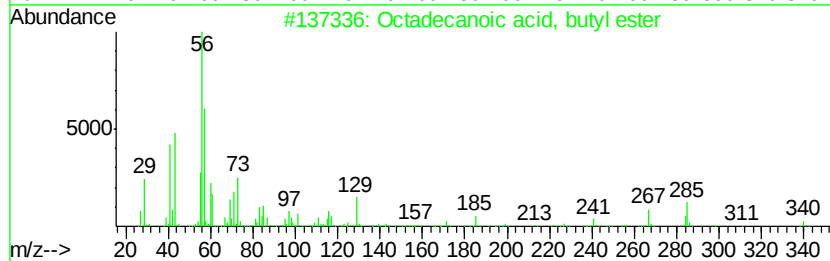
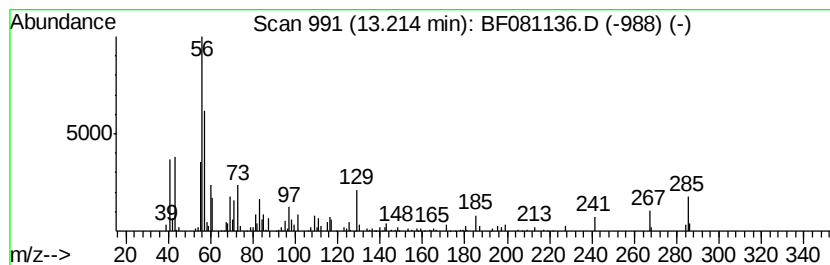
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.21	4.60 ng	125194	Chrysene-d12	13.69	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	83
2	n-Butyl myristate	284	C18H36O2	000110-36-1	80
3	4-Ethyl-4-methyl-5-methylene-[1,...	142	C7H10O3	080956-52-1	35
4	2-Methyl-1-octadecene	266	C19H38	061868-20-0	35
5	Cyclohexane, (1,1-dimethylethyl)-	140	C10H20	003178-22-1	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082015\
Data File : BF081136.D
Acq On : 20 Aug 2015 21:13
Operator : UM/IZ
Sample : G3282-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

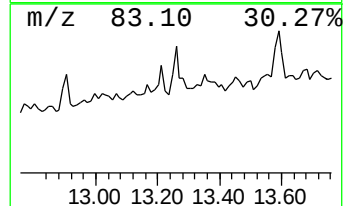
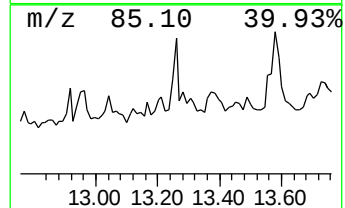
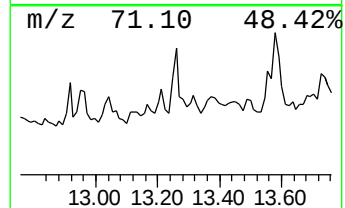
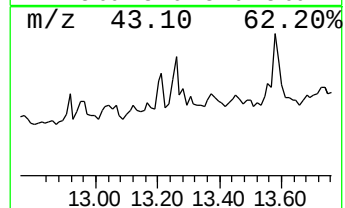
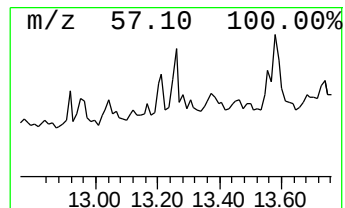
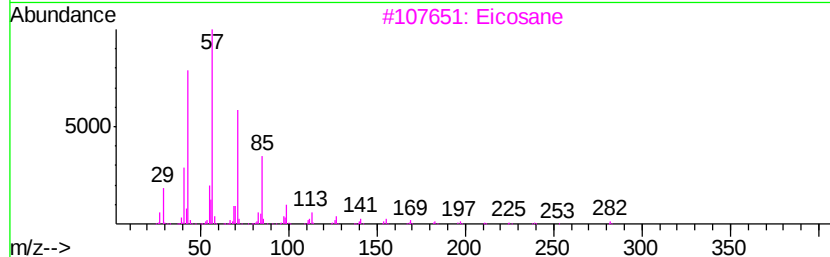
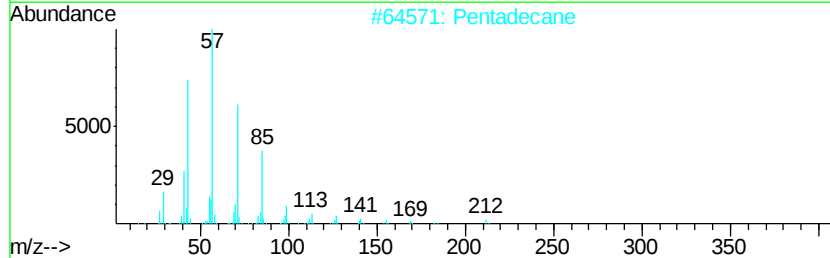
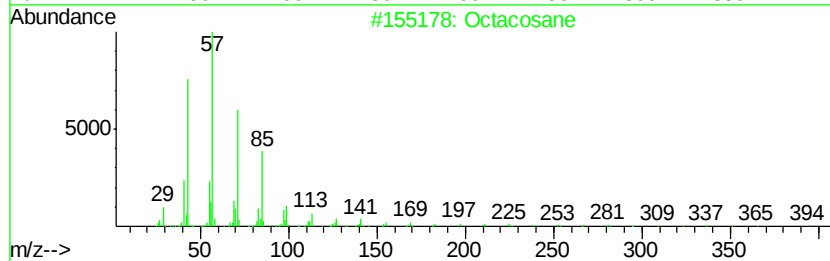
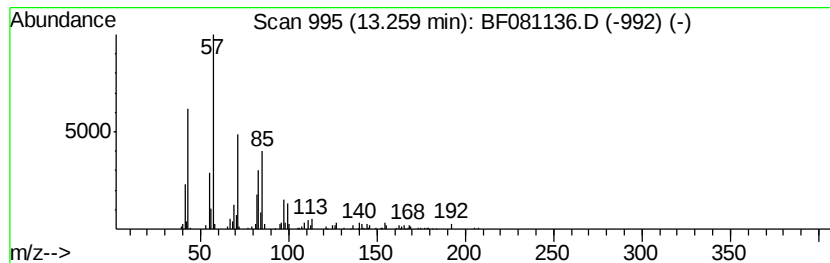
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.26	4.21 ng	114738	Chrysene-d12	13.69
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octacosane	394 C28H58	000630-02-4	72
2	Pentadecane	212 C15H32	000629-62-9	64
3	Eicosane	282 C20H42	000112-95-8	64
4	Tetratetracontane	619 C44H90	007098-22-8	58
5	Heptacosane	380 C27H56	000593-49-7	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082015\
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Acq On : 20 Aug 2015 21:13
Operator : UM/IZ
Sample : G3282-07
Misc :
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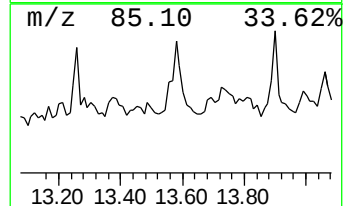
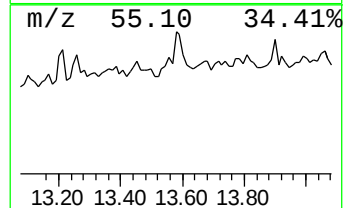
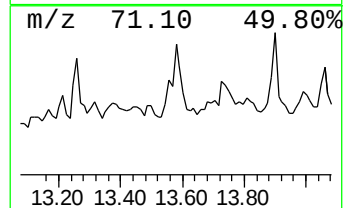
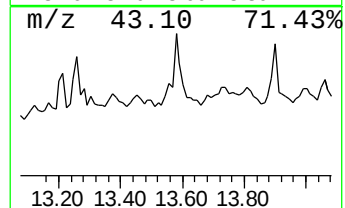
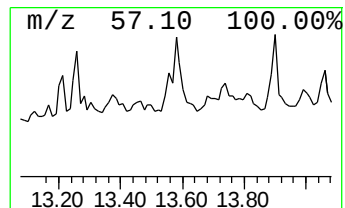
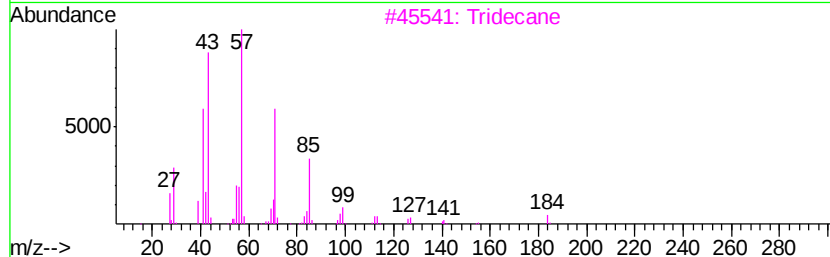
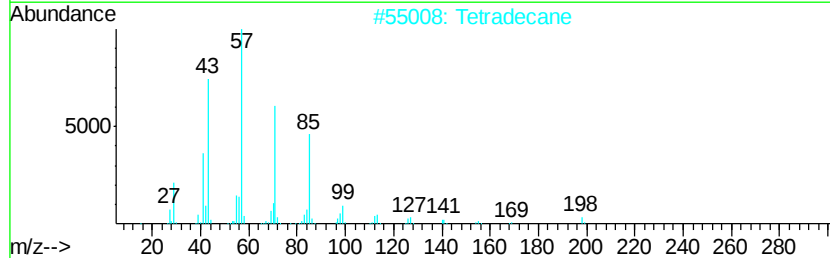
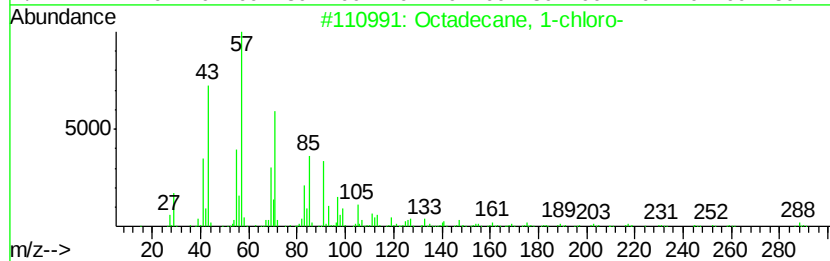
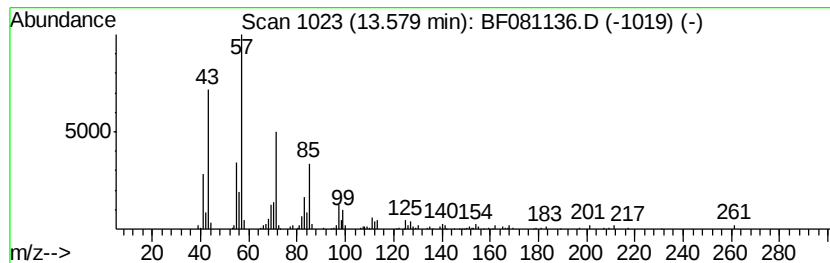
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octadecane, 1-chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.58	8.00 ng	217794	Chrysene-d12	13.69	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	86
2	Tetradecane	198	C14H30	000629-59-4	83
3	Tridecane	184	C13H28	000629-50-5	80
4	Dodecane	170	C12H26	000112-40-3	80
5	Eicosane	282	C20H42	000112-95-8	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082015\
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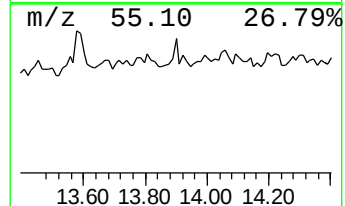
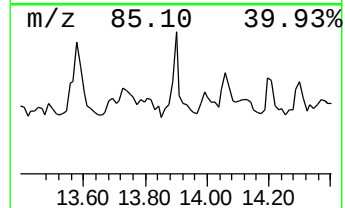
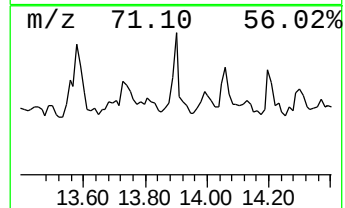
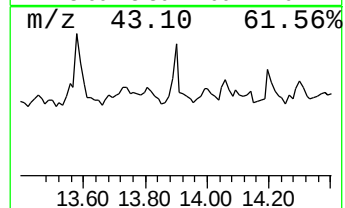
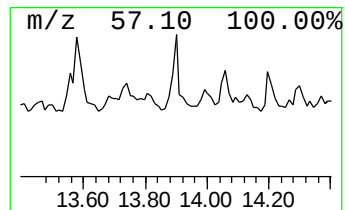
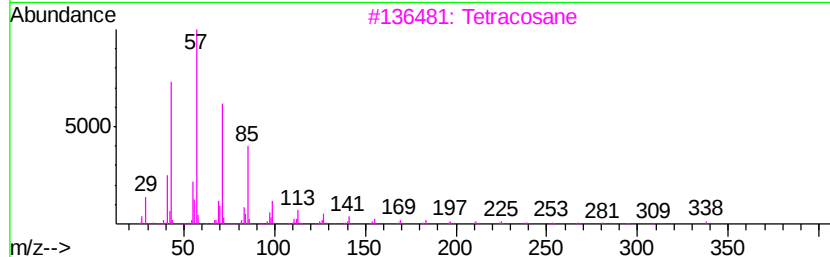
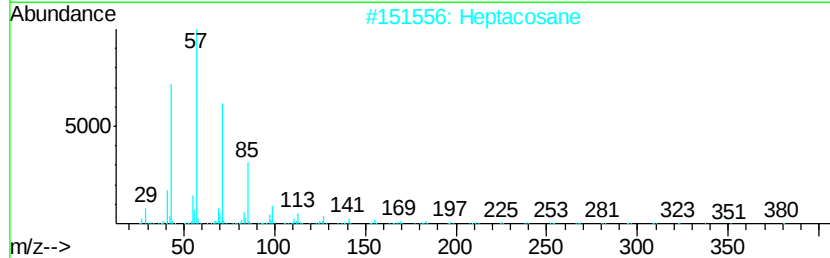
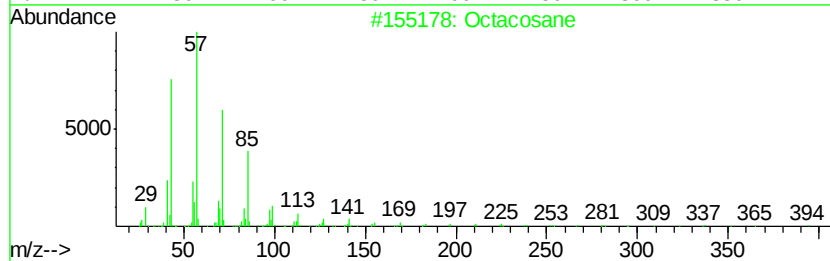
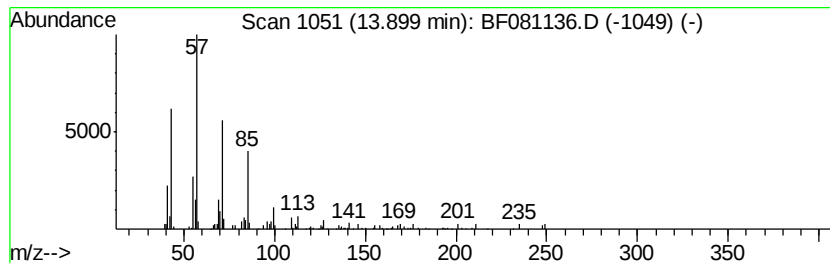
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heptacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.		
13.90	2.79 ng	76032	Chrysene-d12		13.69		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	87
2			Heptacosane	380	C27H56	000593-49-7	87
3			Tetracosane	338	C24H50	000646-31-1	86
4			Tetratetracontane	619	C44H90	007098-22-8	86
5			Octadecane	254	C18H38	000593-45-3	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082015\
Data File : BF081136.D
Acq On : 20 Aug 2015 21:13
Operator : UM/IZ
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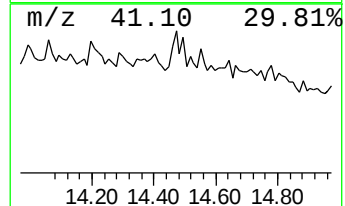
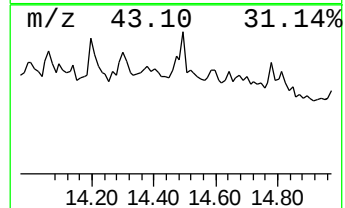
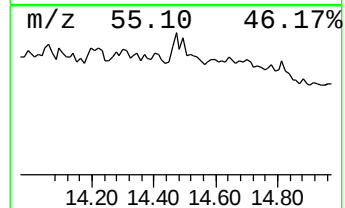
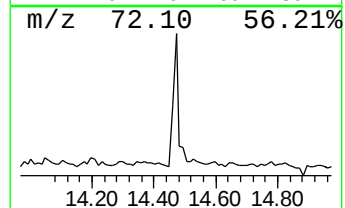
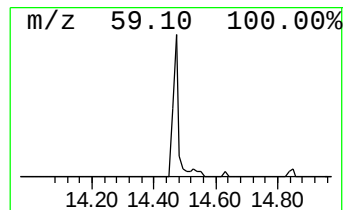
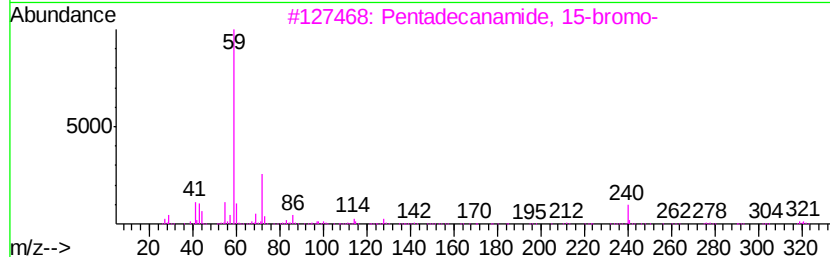
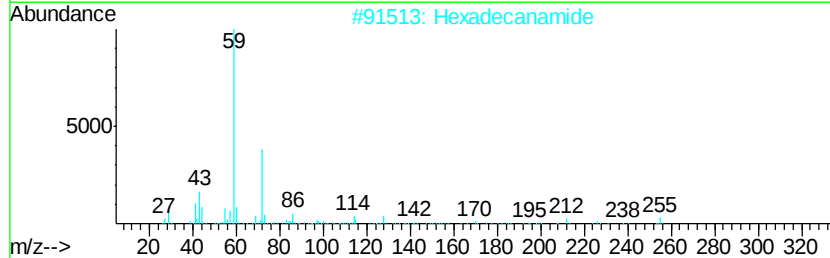
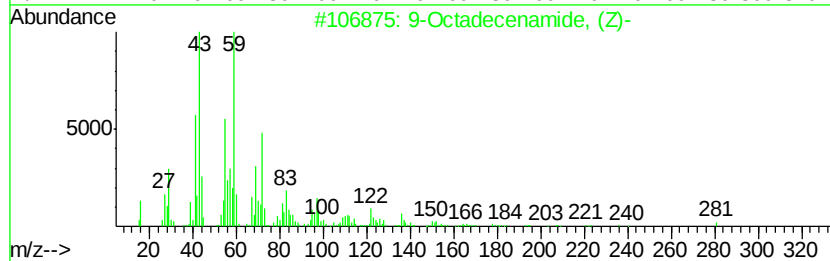
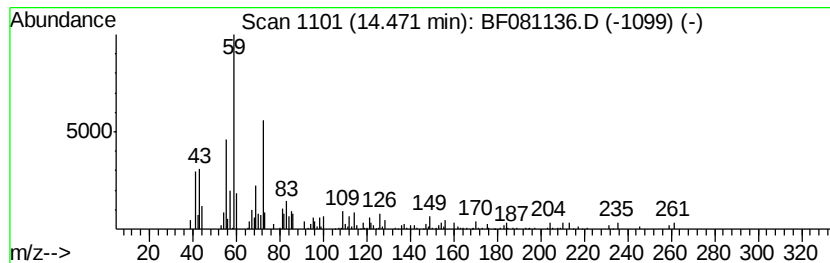
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	4.70 ng	79771	Perylene-d12	15.04

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	64
2			Hexadecanamide	255	C16H33NO	000629-54-9	59
3			Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	59
4			Dodecanamide	199	C12H25NO	001120-16-7	50
5			d-Glucosamine	179	C6H13NO5	000090-77-7	45



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082015\
Data File : BF081136.D
Acq On : 20 Aug 2015 21:13
Operator : UM/IZ
Sample : G3282-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB04-4.0-5.0-081115

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.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-2-one, 4...	3.96	4.0	ng	96413	1	6.57	476360	20.0
2-Pentanone, 4-hy...	4.71	90.8	ng	2162110	1	6.57	476360	20.0
2-Pentanone, 4-me...	5.57	3.4	ng	80385	1	6.57	476360	20.0
unknown6.34	6.34	96.7	ng	2303450	1	6.57	476360	20.0
Hexadecanoic acid...	12.51	6.0	ng	164216	5	13.69	544791	20.0
11-Tricosene	12.59	2.6	ng	69760	5	13.69	544791	20.0
Docosane	12.95	2.2	ng	60802	5	13.69	544791	20.0
Octadecanoic acid...	13.21	4.6	ng	125194	5	13.69	544791	20.0
Octacosane	13.26	4.2	ng	114738	5	13.69	544791	20.0
Octadecane, 1-chl...	13.58	8.0	ng	217794	5	13.69	544791	20.0
Heptacosane	13.90	2.8	ng	76032	5	13.69	544791	20.0
9-Octadecenamide, ...	14.47	4.7	ng	79771	6	15.04	339118	20.0