

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072216\
 Data File : BF089188.D
 Acq On : 22 Jul 2016 10:41
 Operator : UM/SJ
 Sample : H4074-02
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-06-COMP

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-BF072016.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.724	10	12	60	rVB	939037	2413879	100.00%	14.639%
2	4.730	272	275	290	rBV	42919	80385	3.33%	0.488%
3	5.176	312	314	340	rBV	817487	1419046	58.79%	8.606%
4	6.250	406	408	416	rBV	1006671	1452485	60.17%	8.809%
5	6.364	416	418	420	rBV	1353660	1524553	63.16%	9.246%
6	6.593	436	438	449	rVB	221683	274179	11.36%	1.663%
7	6.742	449	451	454	rBV	944849	1044071	43.25%	6.332%
8	7.165	485	488	490	rBV	807424	963166	39.90%	5.841%
9	7.873	548	550	561	rBV	421342	406375	16.83%	2.465%
10	8.948	642	644	647	rBV	1151943	1591675	65.94%	9.653%
11	9.348	677	679	682	rBV	422065	469475	19.45%	2.847%
12	9.622	700	703	705	rBV	357303	445842	18.47%	2.704%
13	10.411	769	772	774	rBV	696467	993550	41.16%	6.026%
14	10.559	781	785	789	rVB2	18182	33812	1.40%	0.205%
15	11.096	829	832	834	rBV	312995	447988	18.56%	2.717%
16	11.508	864	868	870	rVB	109180	103339	4.28%	0.627%
17	11.645	876	880	884	rBV2	24357	39012	1.62%	0.237%
18	12.182	925	927	935	rBV2	295967	536929	22.24%	3.256%
19	12.296	935	937	939	rVB	51139	50744	2.10%	0.308%
20	12.422	945	948	954	rBV	28158	50515	2.09%	0.306%
21	12.674	967	970	973	rBV	1389196	1354504	56.11%	8.215%
22	13.154	1008	1012	1014	rBV	31664	38997	1.62%	0.237%
23	13.599	1047	1051	1057	rBV2	19228	42351	1.75%	0.257%
24	13.714	1058	1061	1063	rBV	269308	358687	14.86%	2.175%
25	14.491	1126	1129	1131	rBV	19505	28562	1.18%	0.173%
26	14.571	1134	1136	1137	rVV	27732	36886	1.53%	0.224%
27	14.651	1140	1143	1145	rVV	22579	27833	1.15%	0.169%
28	15.051	1176	1178	1181	rBV	197998	227035	9.41%	1.377%
29	16.514	1303	1306	1311	rVB	15808	32962	1.37%	0.200%

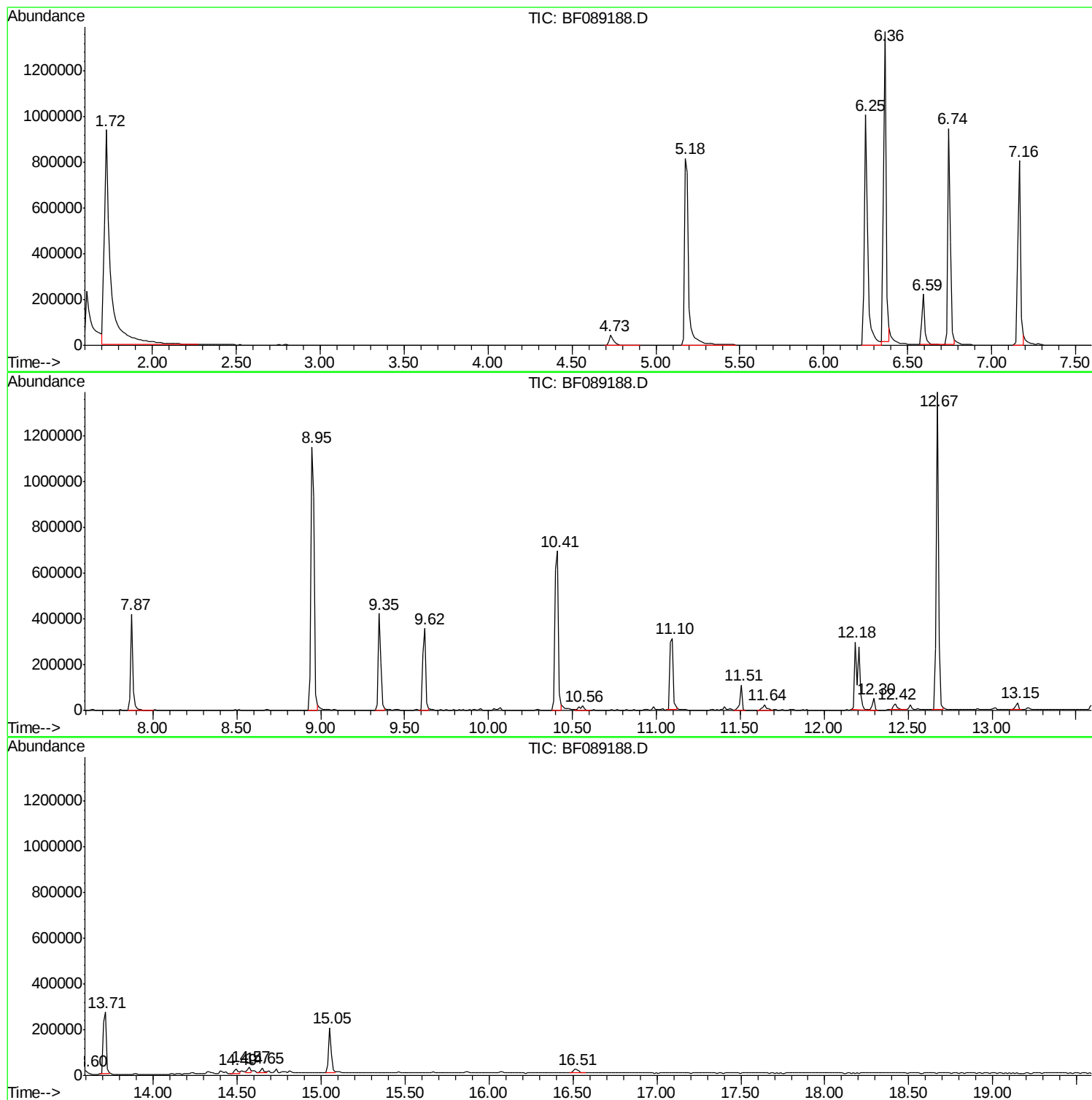
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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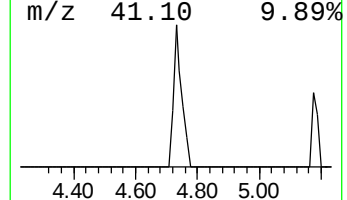
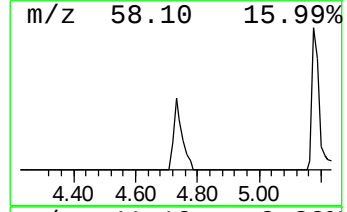
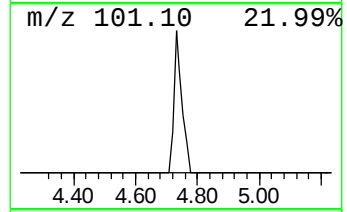
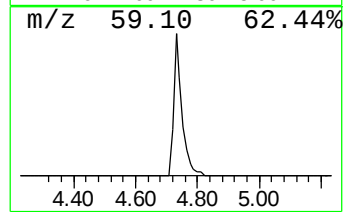
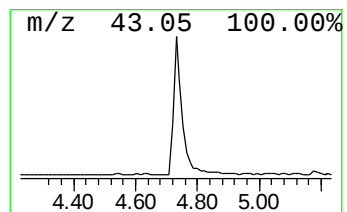
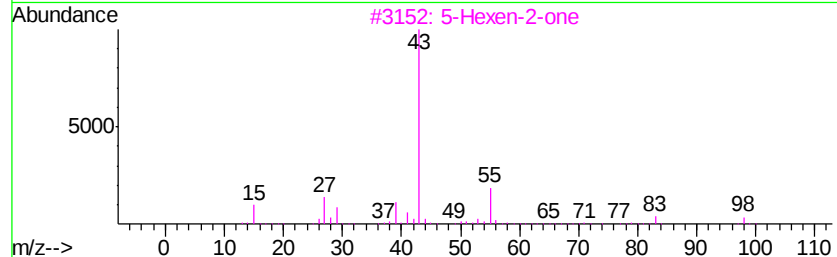
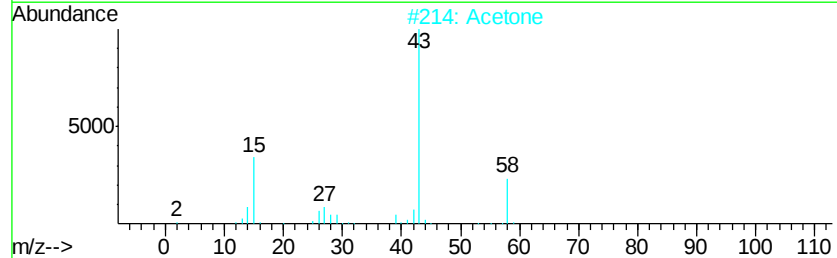
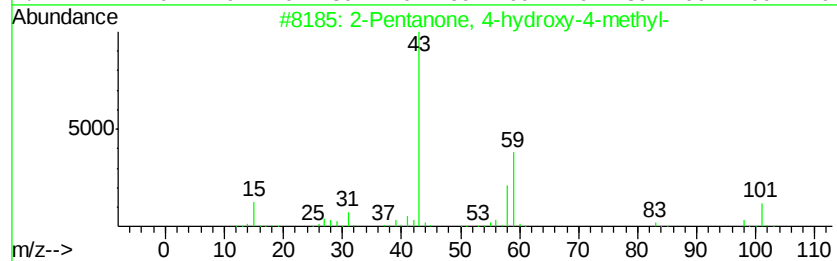
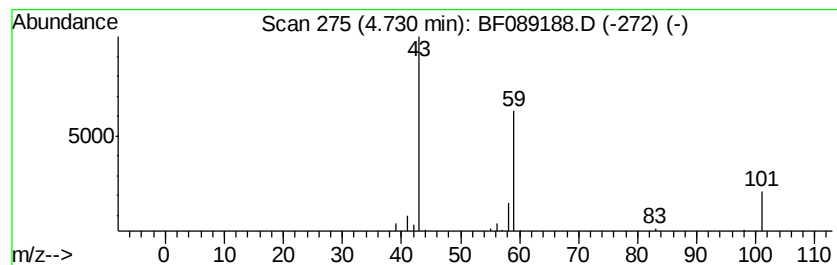
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.73	5.86 ng	80385	1,4-Dichlorobenzene-d4	6.59

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	56
2	Acetone	58	C3H6O		000067-64-1	9
3	5-Hexen-2-one	98	C6H10O		000109-49-9	9
4	3-Hexanol, 4-methyl-	116	C7H16O		000615-29-2	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2		000540-88-5	9



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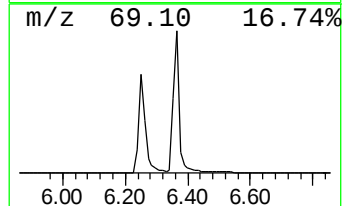
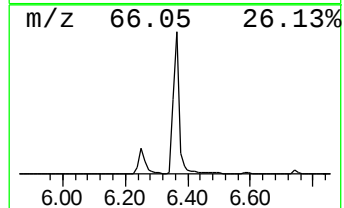
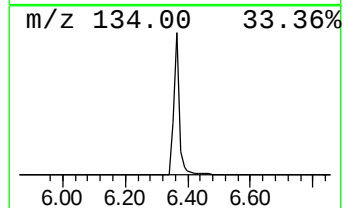
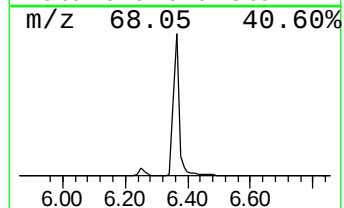
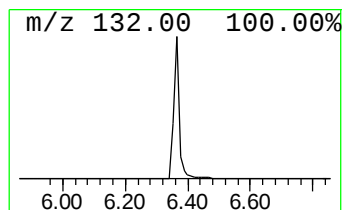
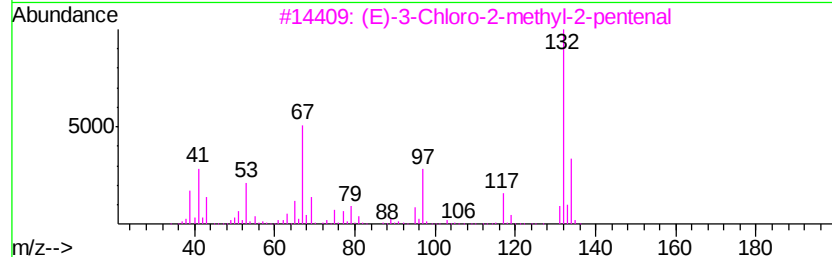
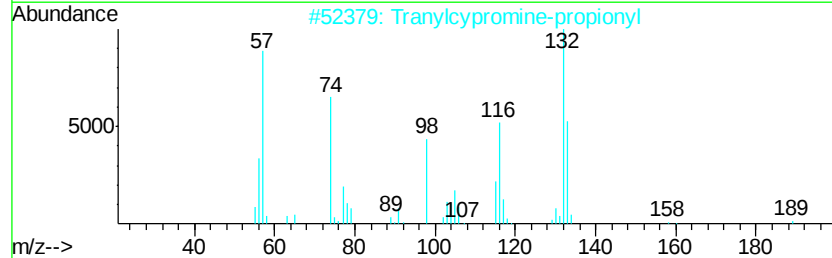
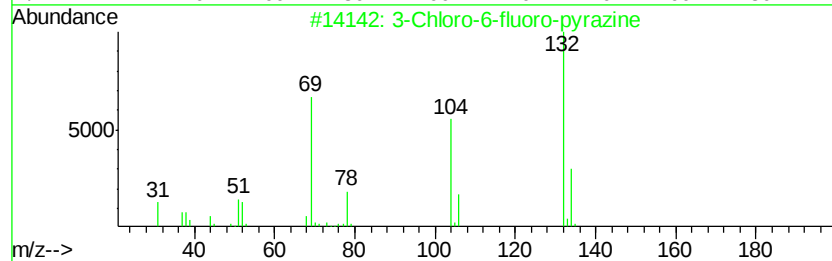
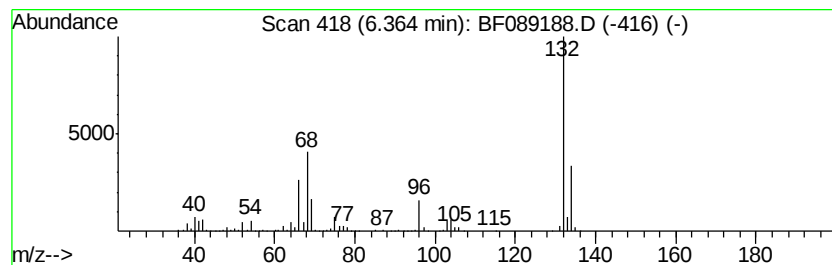
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Peak Number 3 unknown6.36 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	111.21 ng	1524550	1,4-Dichlorobenzene-d4	6.59

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5			1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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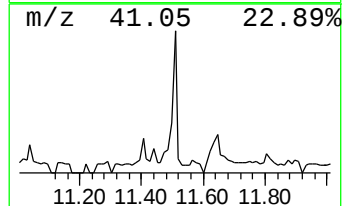
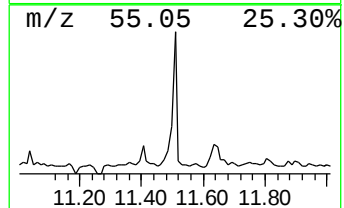
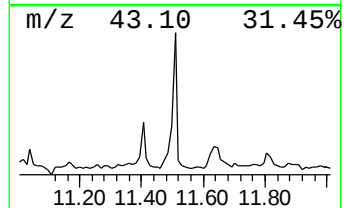
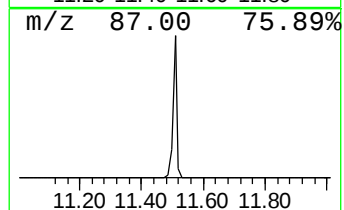
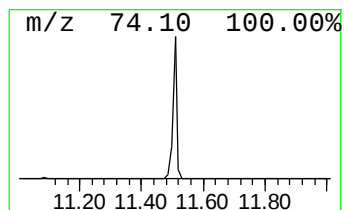
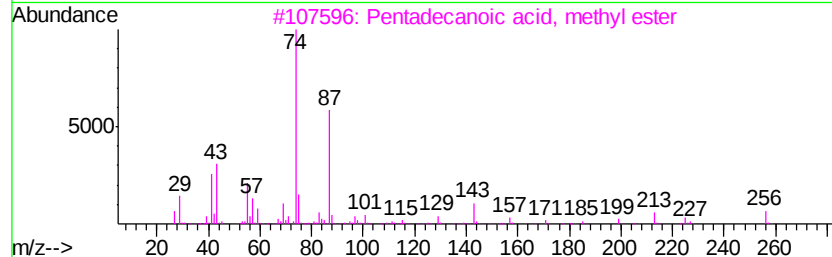
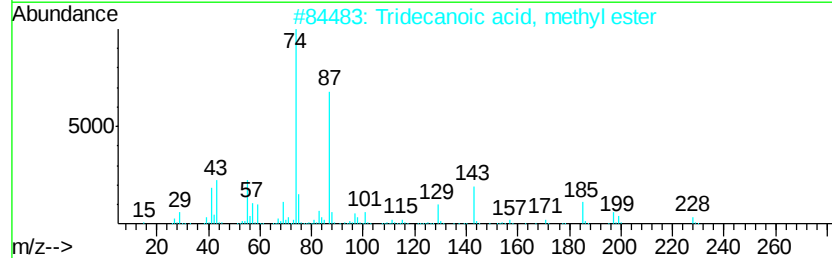
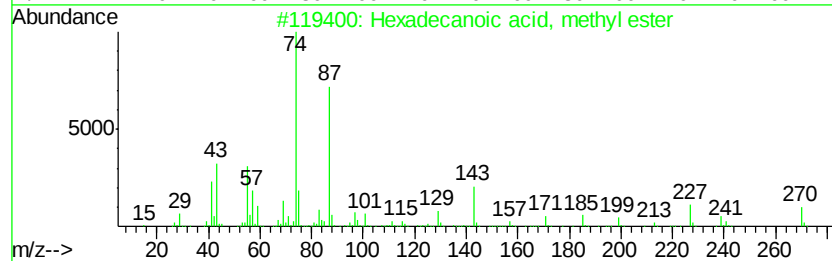
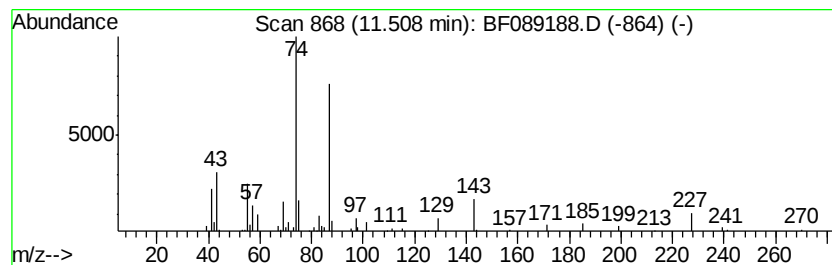
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Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.51	4.61 ng	103339	Phenanthrene-d10	11.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	94
2		Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	87
3		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
4		Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	83
5		Methyl tetradecanoate	242	C15H30O2	000124-10-7	80



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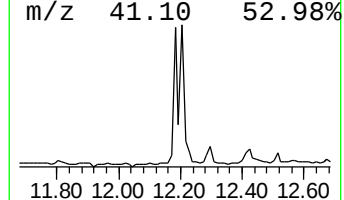
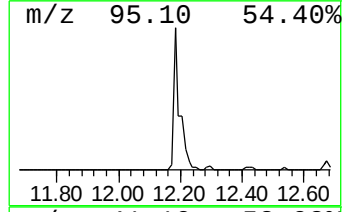
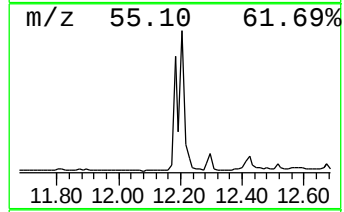
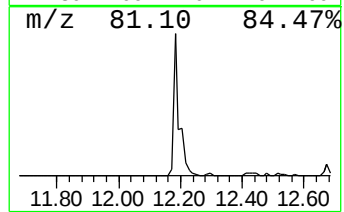
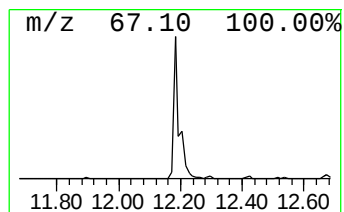
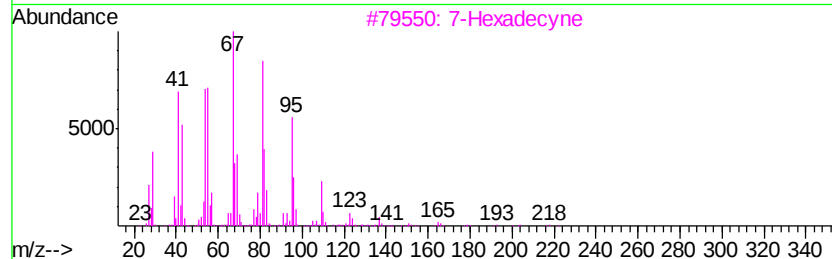
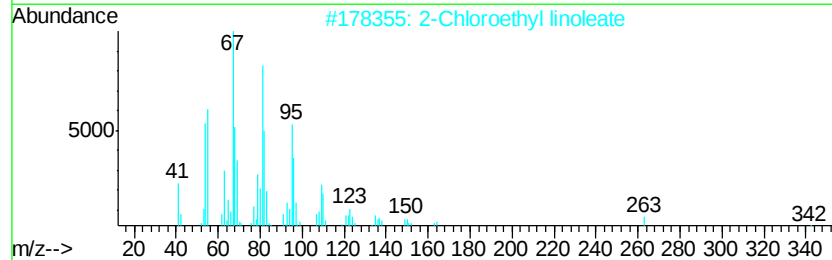
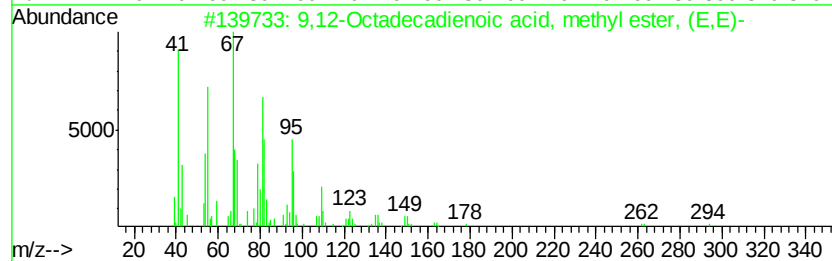
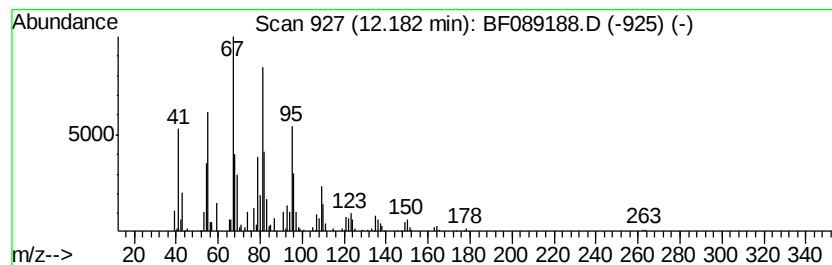
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Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.18	23.97 ng	536929	Phenanthrene-d10	11.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9,12-Octadecadienoic acid, methyl...	294	C19H34O2	002566-97-4	93
2		2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	87
3		7-Hexadecyne	222	C16H30	074685-28-2	83
4		3,4-Octadiene, 7-methyl-	124	C9H16	037050-05-8	83
5		11,14-Eicosadienoic acid, methyl...	322	C21H38O2	002463-02-7	76



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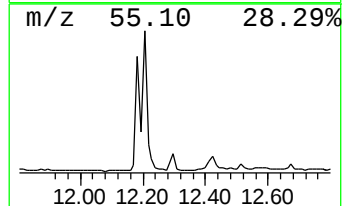
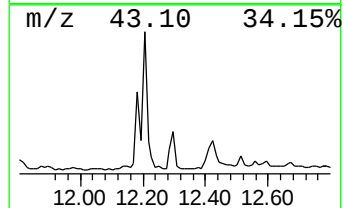
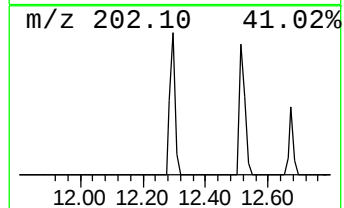
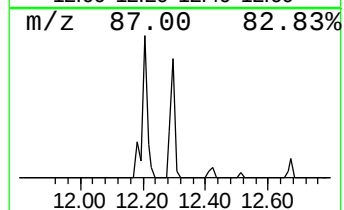
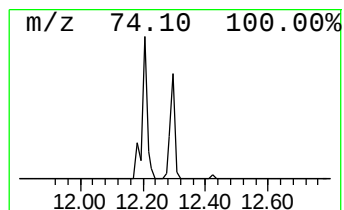
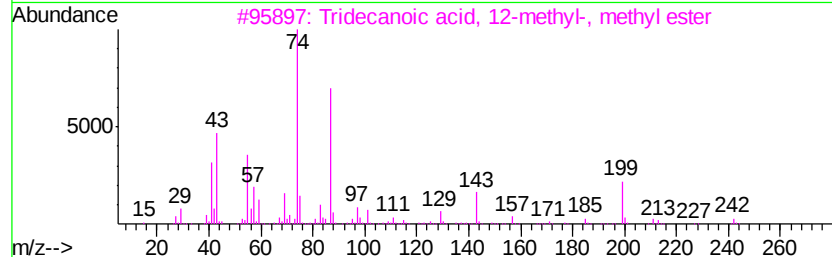
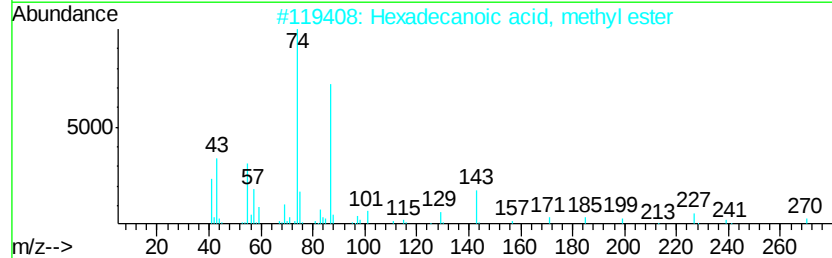
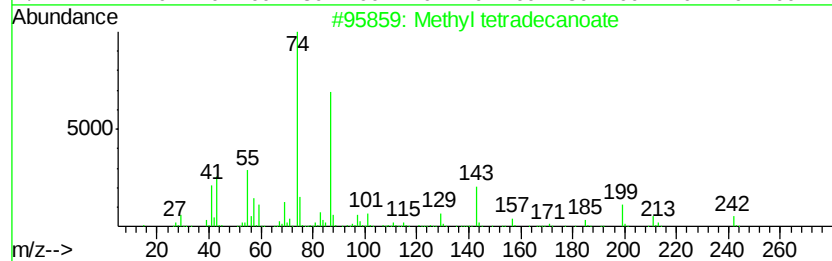
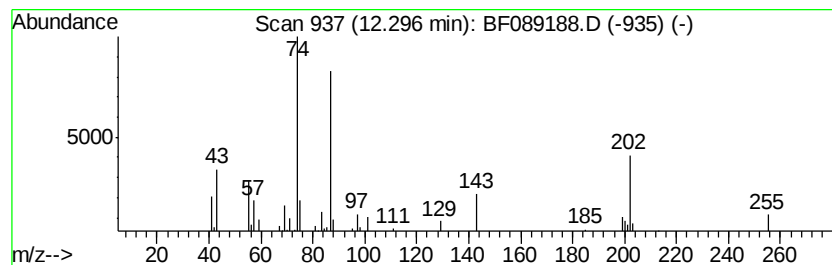
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Peak Number 7 Methyl tetradecanoate Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	2.27 ng	50744	Phenanthrene-d10	11.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	72
2		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	64
3		Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	64
4		Undecanoic acid, 10-methyl-, met...	214	C13H26O2	005129-56-6	59
5		Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	59



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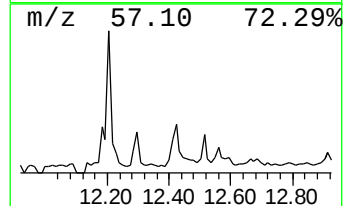
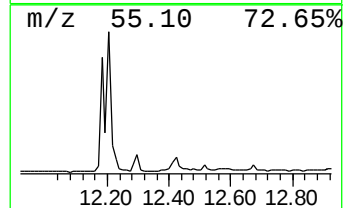
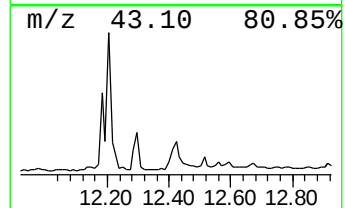
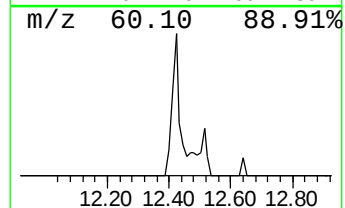
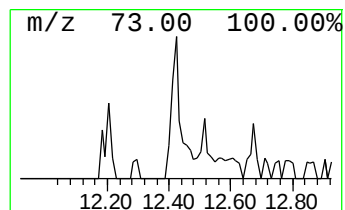
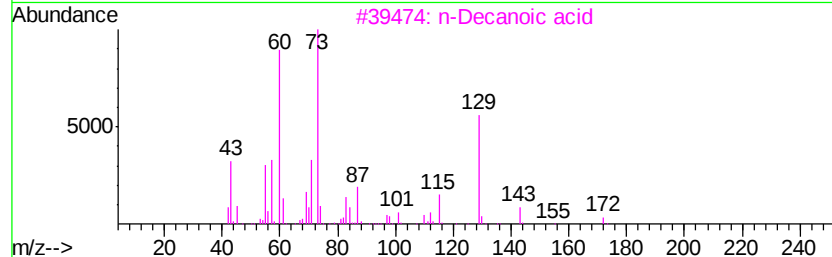
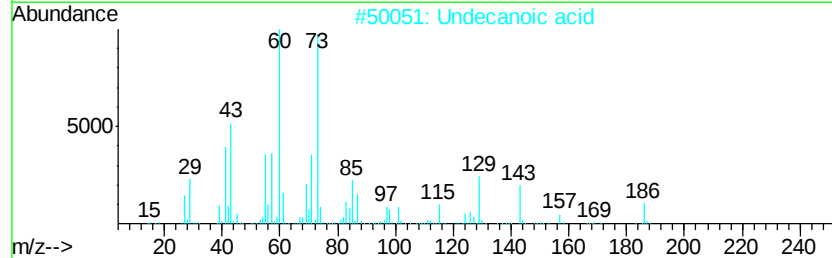
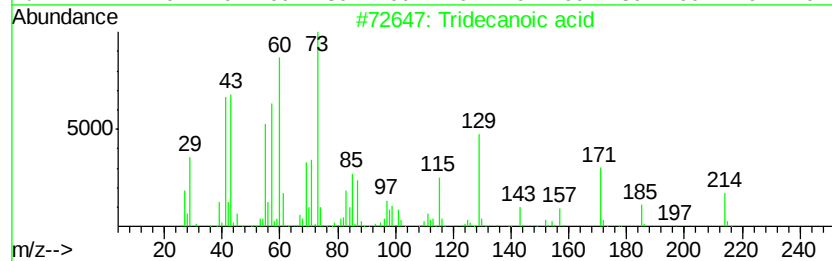
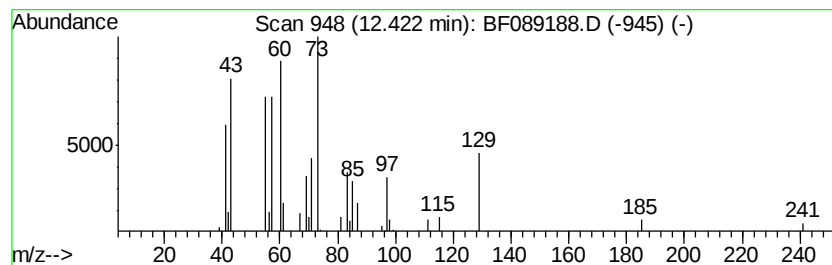
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tridecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.42	2.82 ng	50515	Chrysene-d12	13.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	86
2		Undecanoic acid	186	C11H22O2	000112-37-8	59
3		n-Decanoic acid	172	C10H20O2	000334-48-5	59
4		Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	18
5		Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072216\
Data File : BF089188.D
Acq On : 22 Jul 2016 10:41
Operator : UM/SJ
Sample : H4074-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-06-COMP

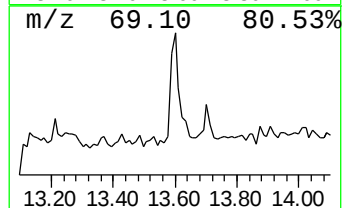
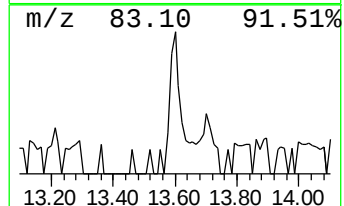
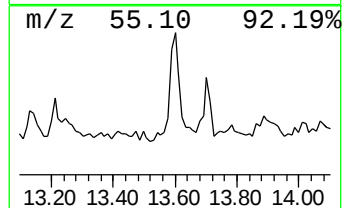
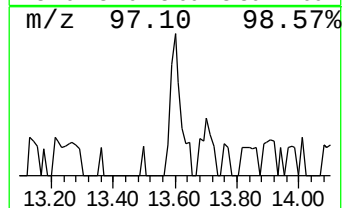
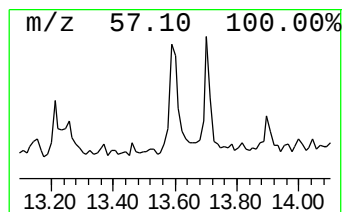
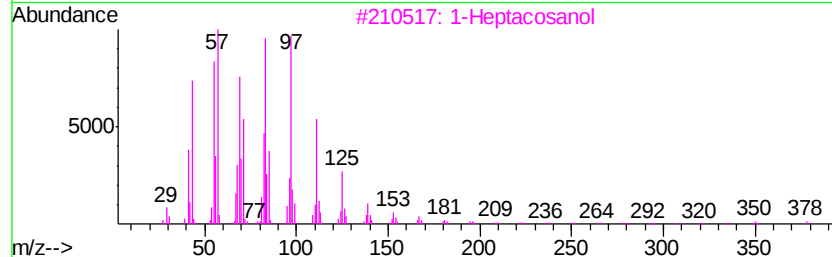
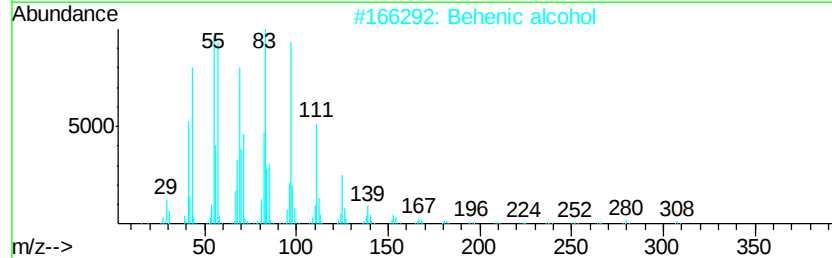
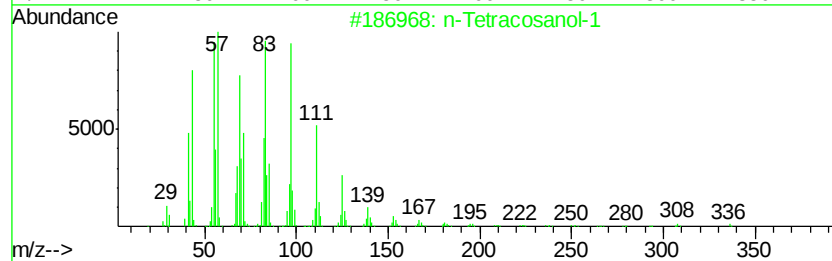
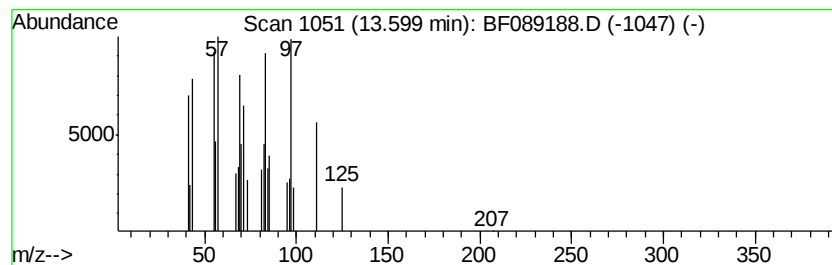
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 n-Tetracosanol-1 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.60	2.36 ng	42351	Chrysene-d12	13.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	91	
2	Behenic alcohol	326	C22H46O	000661-19-8	91	
3	1-Heptacosanol	396	C27H56O	002004-39-9	91	
4	17-Pentatriacontene	491	C35H70	006971-40-0	91	
5	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	90	



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Operator : UM/SJ
Sample : H4074-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-06-COMP

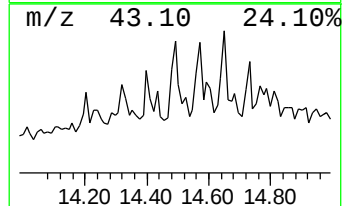
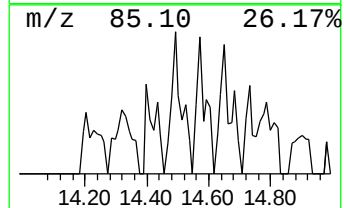
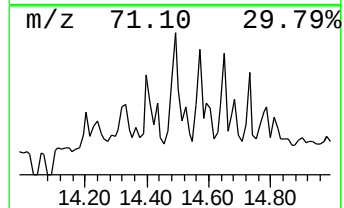
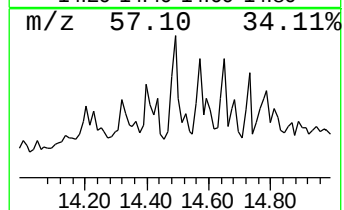
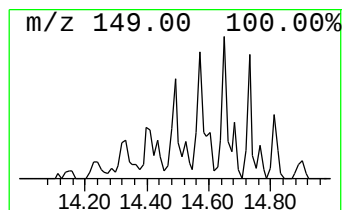
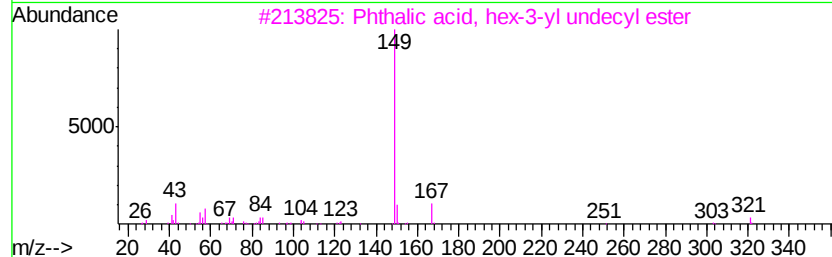
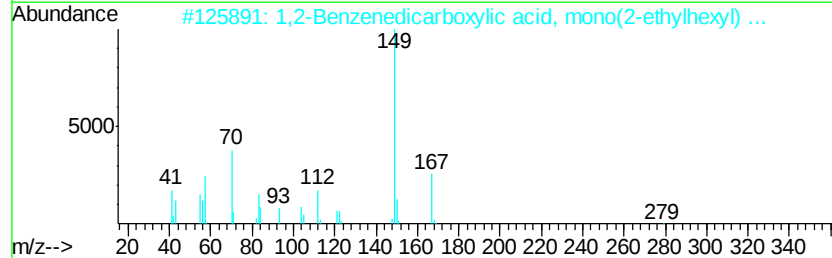
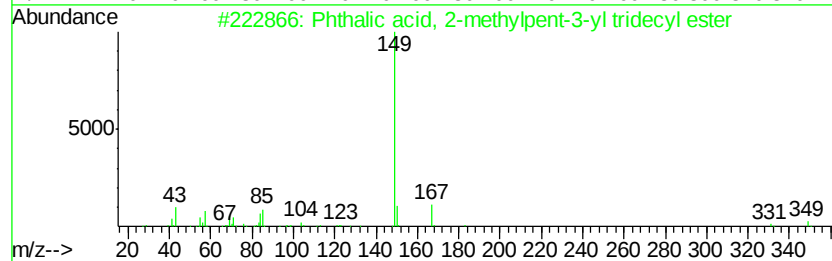
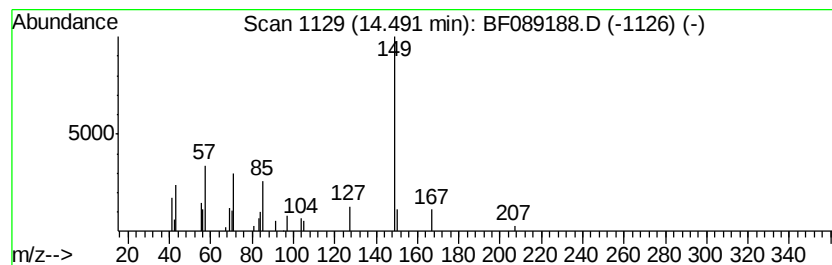
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Phthalic acid, 2-methylpent... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.49	2.52 ng	28562	Perylene-d12	15.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, 2-methylpent-3-yl...	432	C27H44O4	1000356-91-8	50
2		1,2-Benzenedicarboxylic acid, mo...	278	C16H22O4	004376-20-9	47
3		Phthalic acid, hex-3-yl undecyl ...	404	C25H40O4	1000356-96-2	45
4		Phthalic acid, 4-methylpent-2-yl...	376	C23H36O4	1000356-87-9	45
5		Phthalic acid, 5-methylhex-2-yl ...	502	C32H54O4	1000371-07-7	42



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072216\
Data File : BF089188.D
Acq On : 22 Jul 2016 10:41
Operator : UM/SJ
Sample : H4074-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

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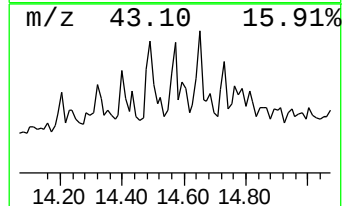
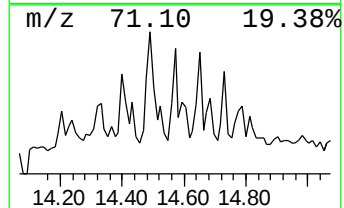
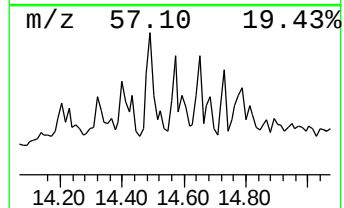
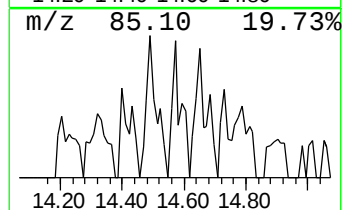
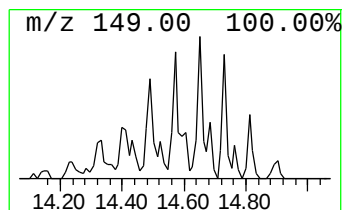
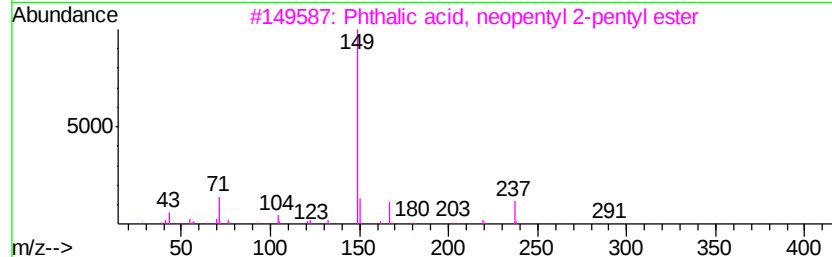
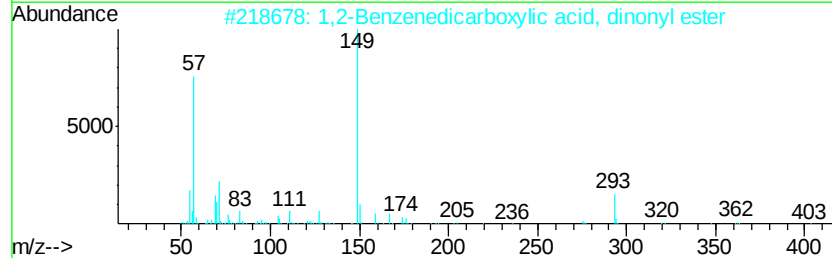
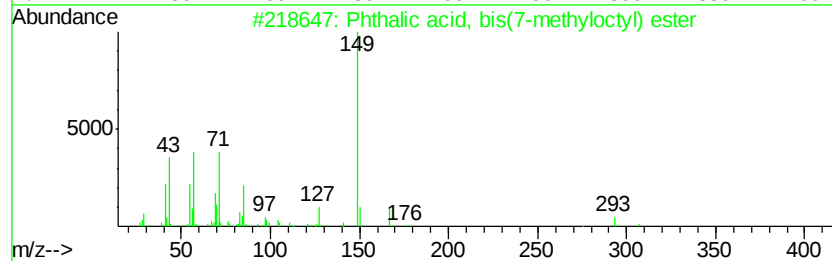
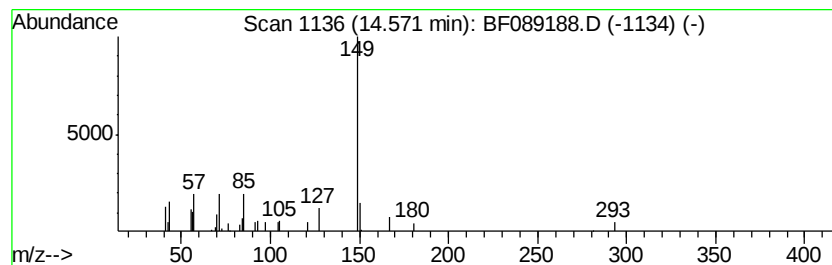
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Phthalic acid, bis(7-methyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	3.25 ng	36886	Perylene-d12	15.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, bis(7-methyloctyl...	418	C26H42O4	020548-62-3	72
2		1,2-Benzenedicarboxylic acid, di...	418	C26H42O4	000084-76-4	64
3		Phthalic acid, neopentyl 2-penty...	306	C18H26O4	1000315-54-0	59
4		Phthalic acid, 2,3-dimethylpheny...	396	C25H32O4	1000357-09-1	59
5		Phthalic acid, 4-isopropylphenyl...	396	C25H32O4	1000315-66-5	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072216\
Data File : BF089188.D
Acq On : 22 Jul 2016 10:41
Operator : UM/SJ
Sample : H4074-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

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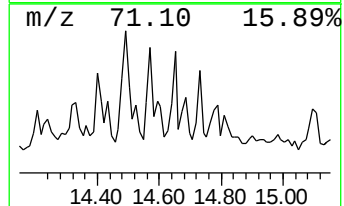
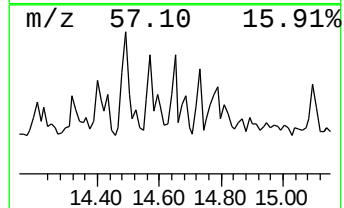
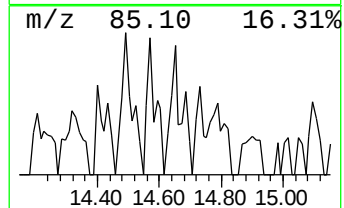
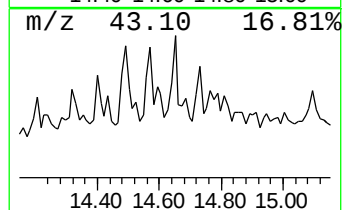
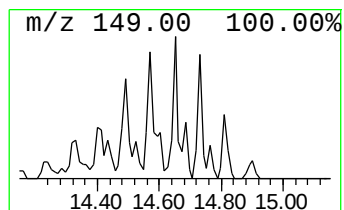
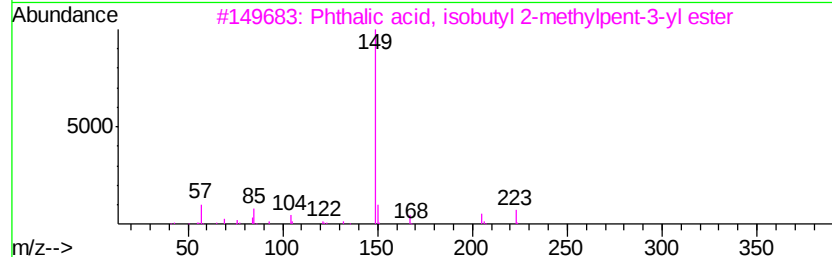
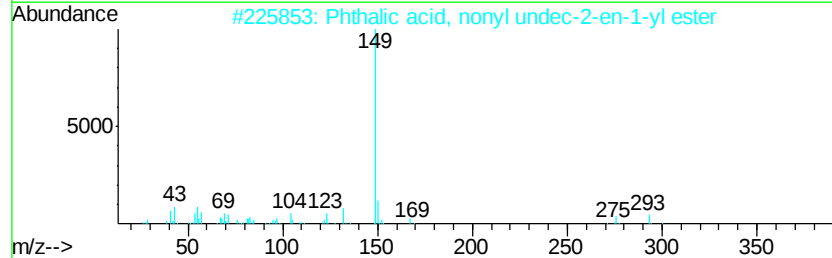
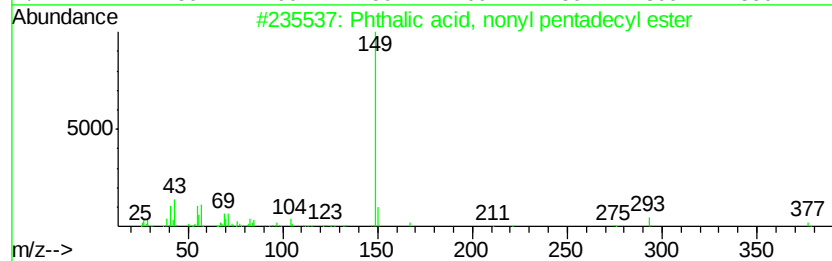
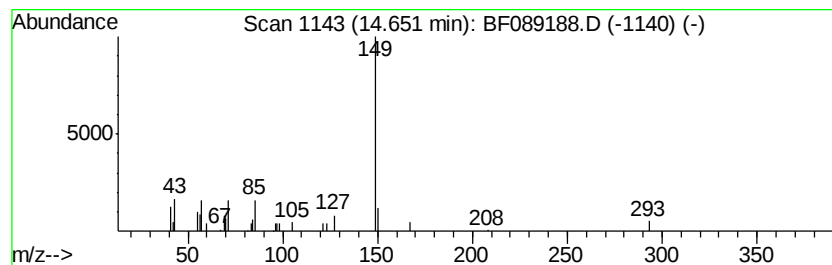
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Phthalic acid, nonyl pentad... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	2.45 ng	27833	Perylene-d12	15.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, nonyl pentadecyl ...	502	C32H54O4	1000308-92-7	72
2		Phthalic acid, nonyl undec-2-en-...	444	C28H44O4	1000315-42-0	64
3		Phthalic acid, isobutyl 2-methyl...	306	C18H26O4	1000356-90-7	64
4		Phthalic acid, hexyl undecyl ester	404	C25H40O4	1000308-91-6	64
5		1,2-Benzenedicarboxylic acid, bu...	362	C22H34O4	000089-18-9	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072216\
Data File : BF089188.D
Acq On : 22 Jul 2016 10:41
Operator : UM/SJ
Sample : H4074-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

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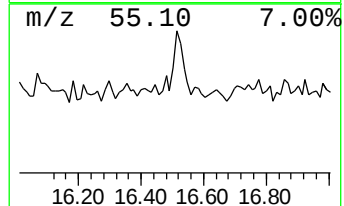
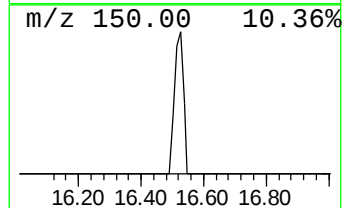
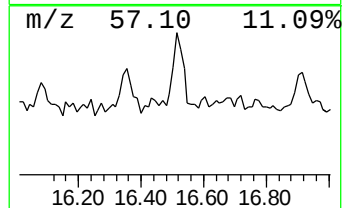
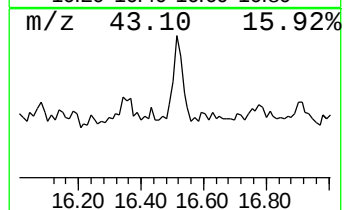
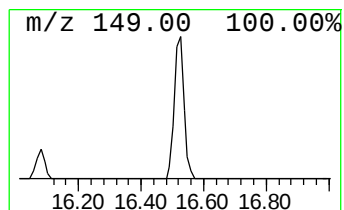
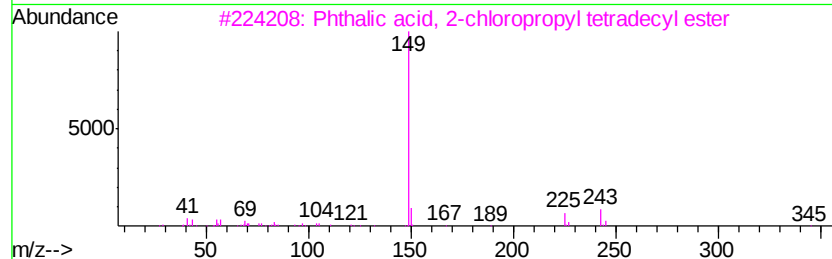
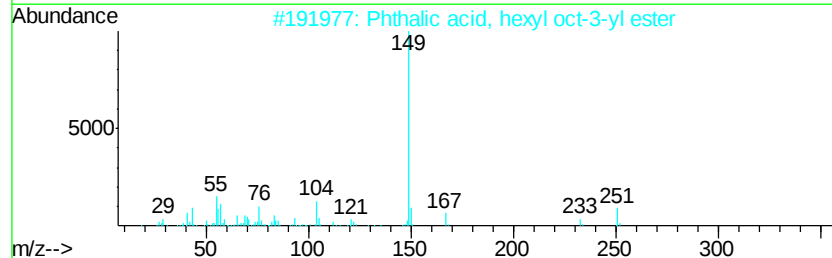
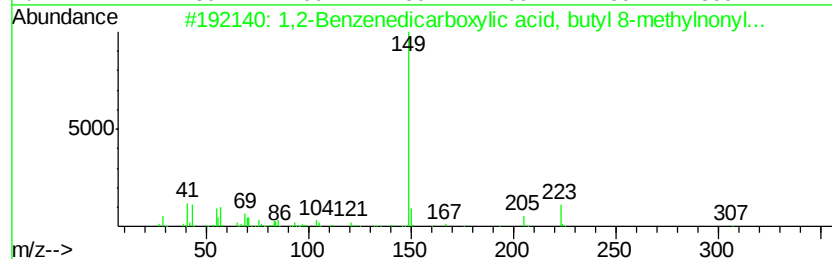
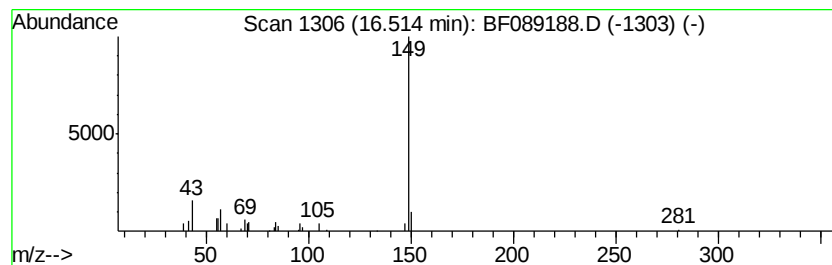
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 1,2-Benzenedicarboxylic aci... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.51	2.90 ng	32962	Perylene-d12	15.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Benzenedicarboxylic acid, bu...	362	C22H34O4	000089-18-9	72
2		Phthalic acid, hexyl oct-3-yl ester	362	C22H34O4	1000377-71-5	72
3		Phthalic acid, 2-chloropropyl te...	438	C25H39ClO4	1000356-83-5	64
4		Phthalic acid, hexyl 6-methylhep...	362	C22H34O4	1000377-96-0	64
5		Phthalic acid, heptyl undecyl ester	418	C26H42O4	1000308-94-0	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072216\
 Data File : BF089188.D
 Acq On : 22 Jul 2016 10:41
 Operator : UM/SJ
 Sample : H4074-02
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-06-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.73	5.9	ng	80385	1	6.59	274179	20.0
unknown6.36	6.36	111.2	ng	1524550	1	6.59	274179	20.0
Hexadecanoic acid...	11.51	4.6	ng	103339	4	11.10	447988	20.0
9,12-Octadecadien...	12.18	24.0	ng	536929	4	11.10	447988	20.0
Methyl tetradecan...	12.30	2.3	ng	50744	4	11.10	447988	20.0
Tridecanoic acid	12.42	2.8	ng	50515	5	13.71	358687	20.0
n-Tetracosanol-1	13.60	2.4	ng	42351	5	13.71	358687	20.0
Phthalic acid, 2-...	14.49	2.5	ng	28562	6	15.05	227035	20.0
Phthalic acid, bi...	14.57	3.3	ng	36886	6	15.05	227035	20.0
Phthalic acid, no...	14.65	2.5	ng	27833	6	15.05	227035	20.0
1,2-Benzenedicarb...	16.51	2.9	ng	32962	6	15.05	227035	20.0