

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031416\
 Data File : BF085421.D
 Acq On : 14 Mar 2016 11:37
 Operator : UM/SJ
 Sample : H1731-24
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-26-COMP

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-BF030316.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.144	247	250	259	rVB	253078	431732	7.46%	0.843%
2	5.544	281	285	287	rBV	4099659	5786828	100.00%	11.304%
3	6.561	371	374	376	rBV	3989565	5071817	87.64%	9.907%
4	6.699	383	386	388	rBV	4728250	5427693	93.79%	10.602%
5	6.927	403	406	408	rBV	1277812	1239694	21.42%	2.422%
6	7.087	417	420	422	rBV	3768105	4371599	75.54%	8.539%
7	7.487	452	455	458	rBV	2700424	3947218	68.21%	7.710%
8	7.579	460	463	465	rVB	71764	92623	1.60%	0.181%
9	8.207	516	518	521	rBV	1791470	1561906	26.99%	3.051%
10	9.293	609	613	615	rBV	4814199	5777517	99.84%	11.286%
11	9.682	644	647	648	rBV	1310086	1174172	20.29%	2.294%
12	9.899	664	666	668	rVB	152701	163440	2.82%	0.319%
13	9.967	670	672	674	rVB	1878480	1698304	29.35%	3.317%
14	10.219	692	694	696	rBV2	48714	58439	1.01%	0.114%
15	10.390	708	709	711	rVB	222025	232435	4.02%	0.454%
16	10.608	726	728	732	rBV	79891	157702	2.73%	0.308%
17	10.756	738	741	744	rBV	3123185	3256818	56.28%	6.362%
18	10.870	749	751	755	rBV	225463	326771	5.65%	0.638%
19	11.065	765	768	772	rBV2	32216	80896	1.40%	0.158%
20	11.316	787	790	791	rBV	161512	145562	2.52%	0.284%
21	11.453	799	802	804	rBV	1579532	1633176	28.22%	3.190%
22	11.499	804	806	810	rVB2	29303	70475	1.22%	0.138%
23	11.796	830	832	834	rBV	74389	89757	1.55%	0.175%
24	11.968	845	847	849	rBV2	172852	224606	3.88%	0.439%
25	12.002	849	850	854	rVB	69247	79456	1.37%	0.155%
26	12.665	906	908	914	rBV2	44235	105029	1.81%	0.205%
27	12.756	914	916	921	rVV	236231	303564	5.25%	0.593%
28	12.859	923	925	926	rVV	105078	149914	2.59%	0.293%
29	12.905	926	929	930	rVV2	35703	88757	1.53%	0.173%
30	12.928	930	931	934	rVB	78067	65678	1.13%	0.128%
31	13.042	938	941	943	rBV	3868981	4555538	78.72%	8.899%
32	13.556	984	986	988	rBV	120891	110828	1.92%	0.216%
33	13.922	1016	1018	1023	rBV2	181835	239004	4.13%	0.467%
34	14.082	1030	1032	1035	rBV	921469	958540	16.56%	1.872%

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Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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35	14.551	1071	1073	1076	rBV	37769	61183	1.06%	0.120%
36	15.545	1157	1160	1171	rVB	728971	1010413	17.46%	1.974%
37	16.059	1201	1205	1208	rBV2	44985	105975	1.83%	0.207%
38	16.242	1219	1221	1228	rVB6	27590	63809	1.10%	0.125%
39	16.448	1234	1239	1241	rBV3	33897	109123	1.89%	0.213%
40	17.568	1333	1337	1342	rBV3	65903	164967	2.85%	0.322%

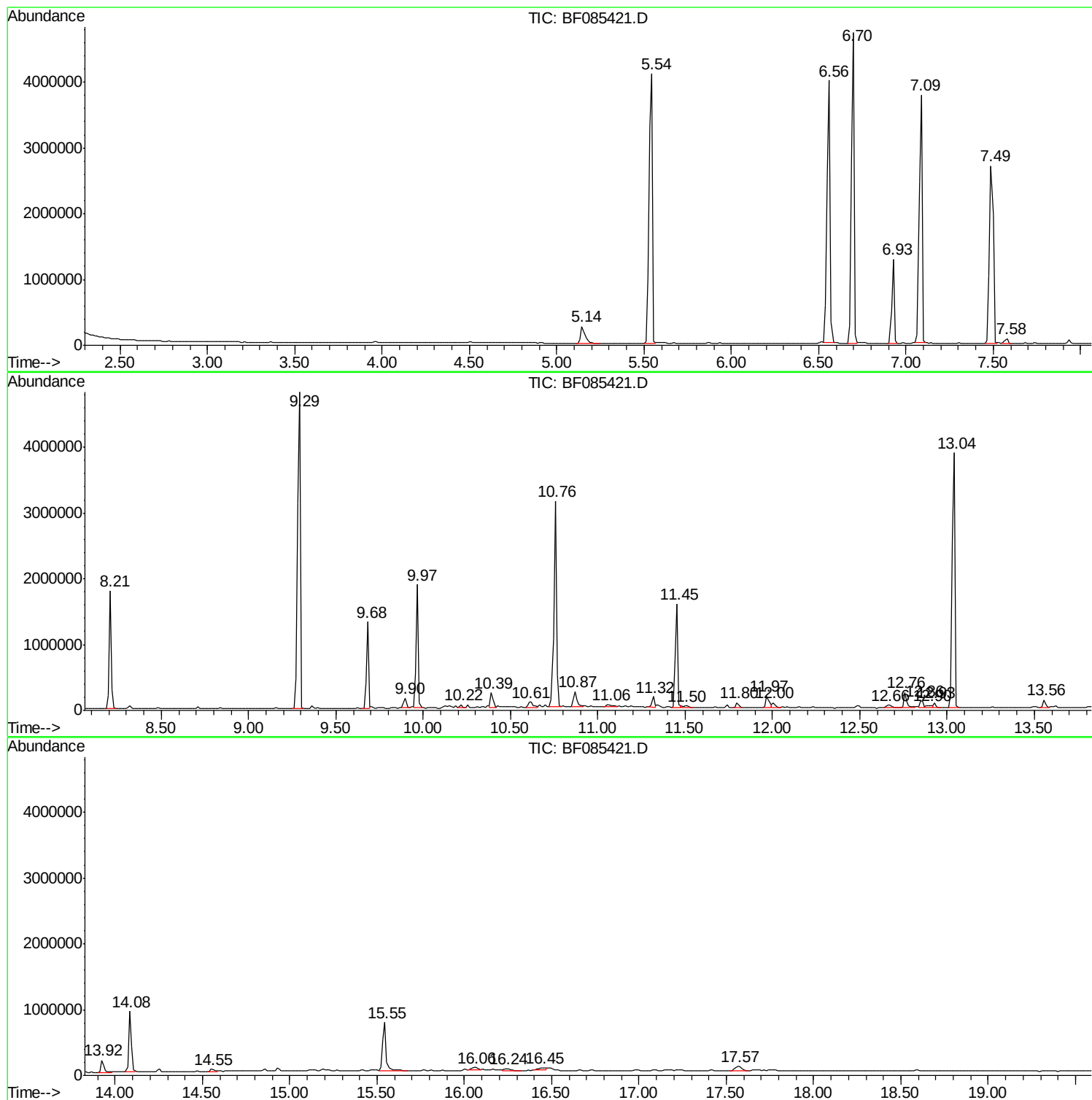
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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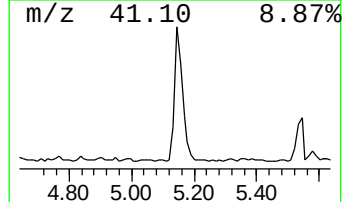
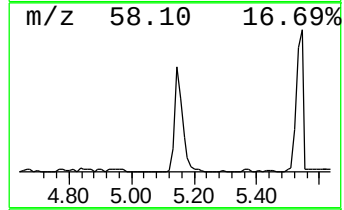
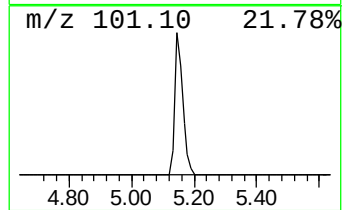
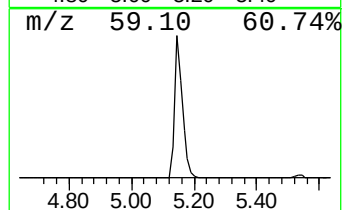
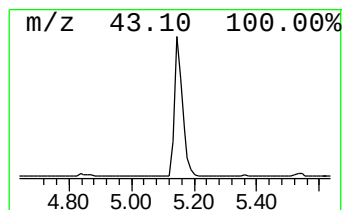
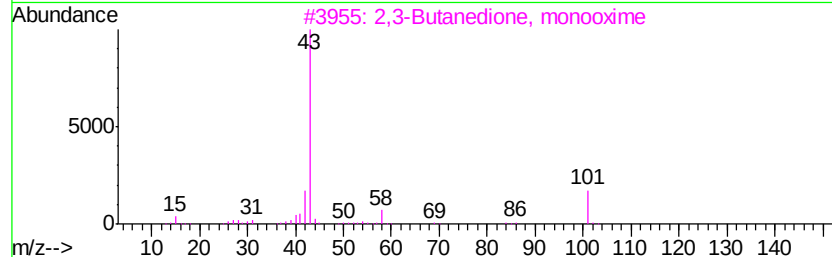
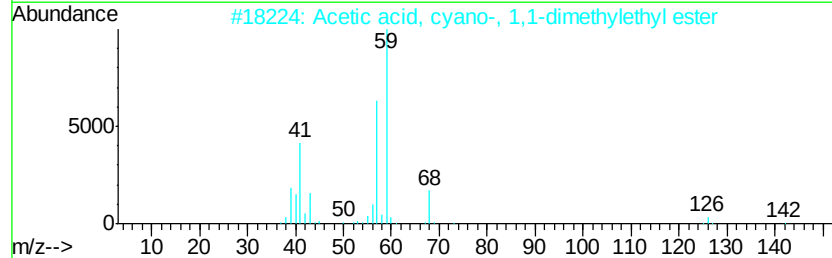
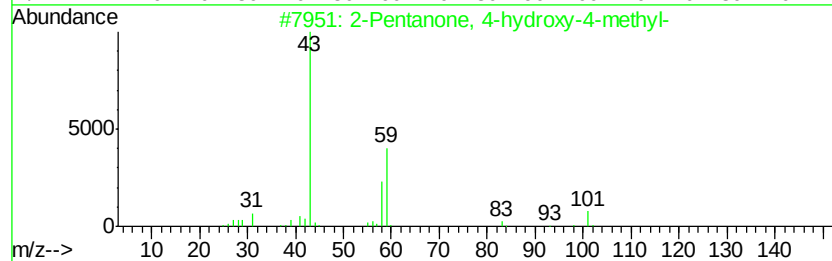
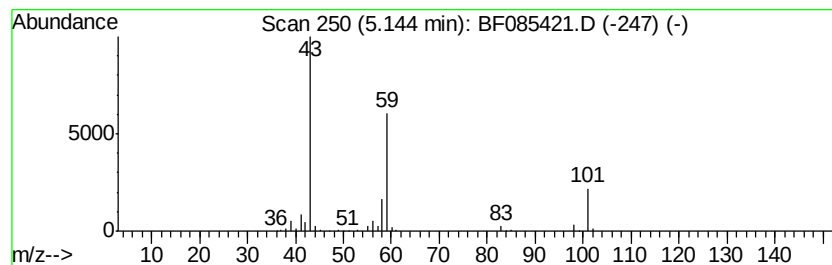
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	6.97 ng	431732	1,4-Dichlorobenzene-d4	6.93

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56	
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32	
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25	
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9	
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9	



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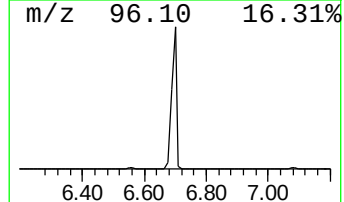
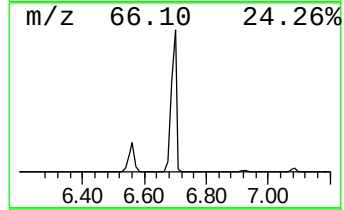
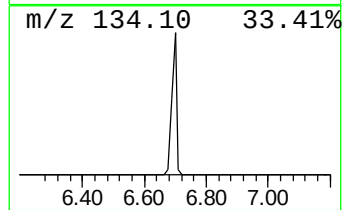
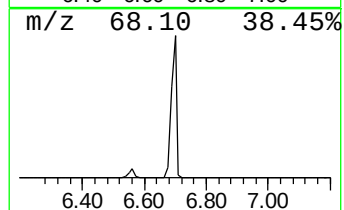
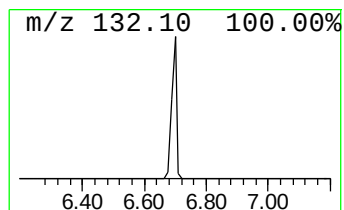
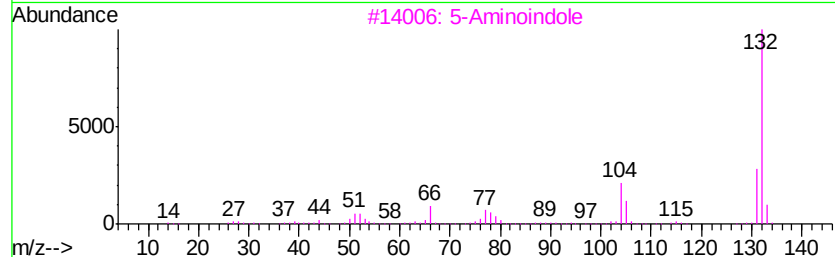
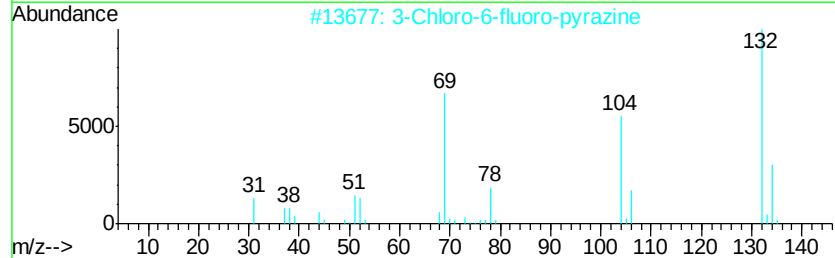
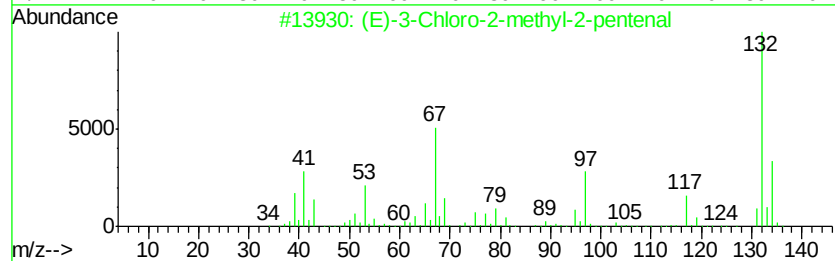
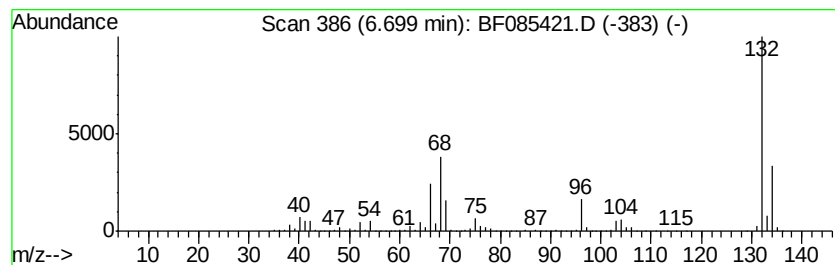
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	87.57 ng	5427690	1,4-Dichlorobenzene-d4	6.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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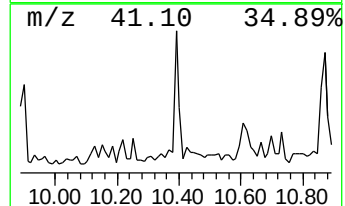
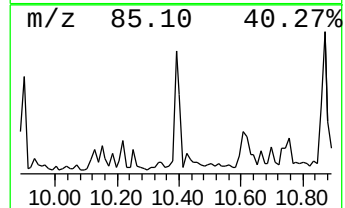
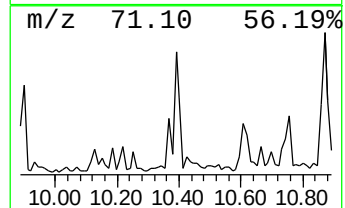
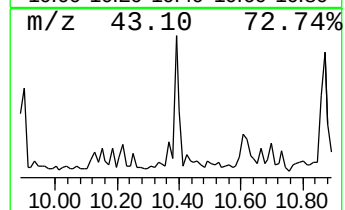
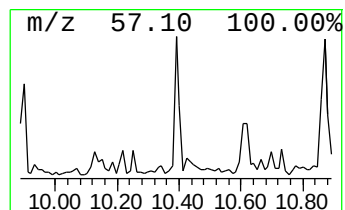
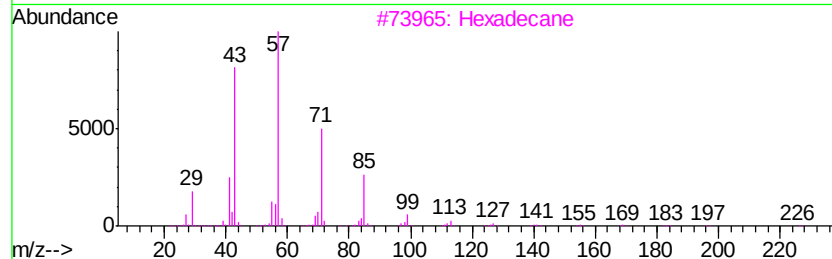
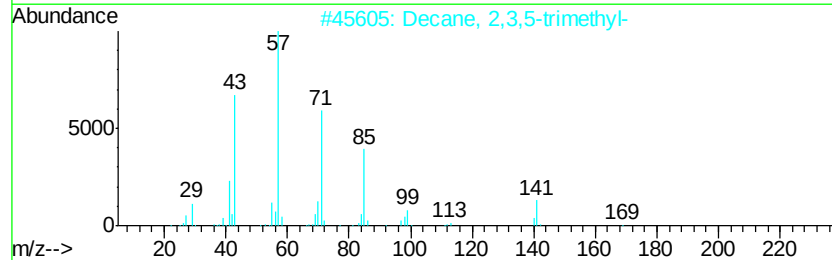
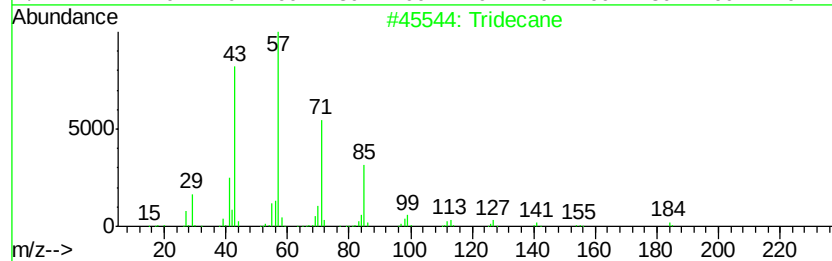
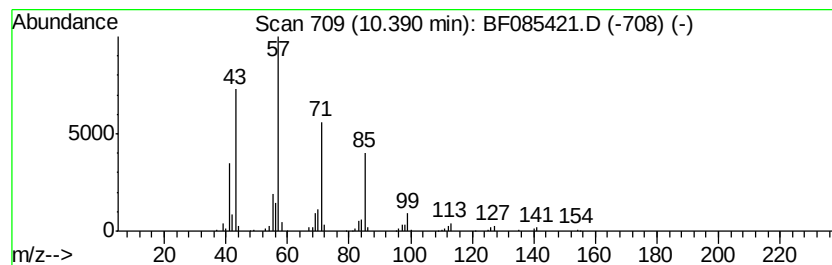
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tridecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.39	2.74 ng	232435	Acenaphthene-d10		9.97
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	86
2	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83
3	Hexadecane	226	C16H34	000544-76-3	80
4	Nonadecane	268	C19H40	000629-92-5	72
5	Tetradecane	198	C14H30	000629-59-4	72



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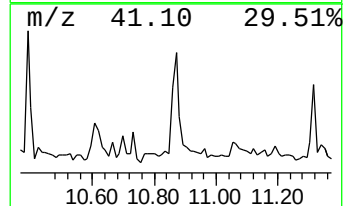
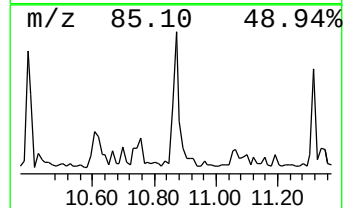
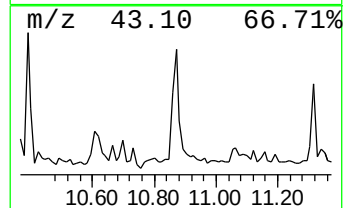
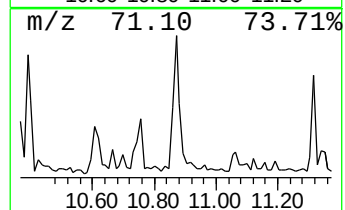
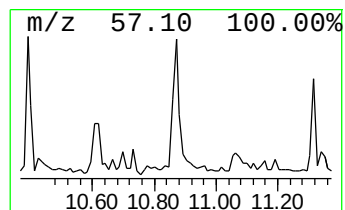
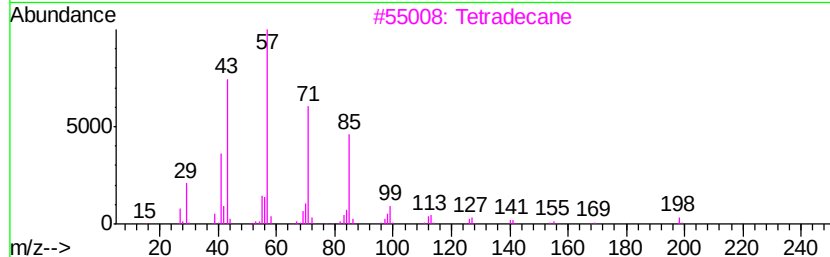
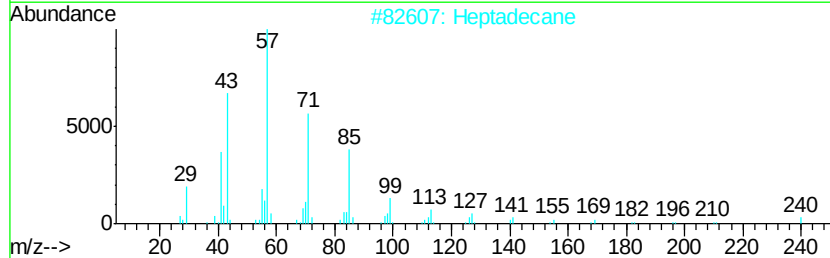
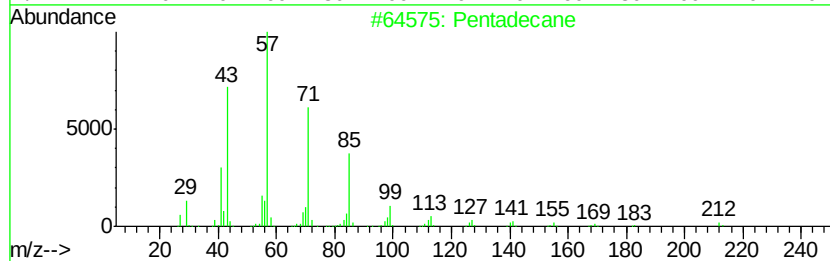
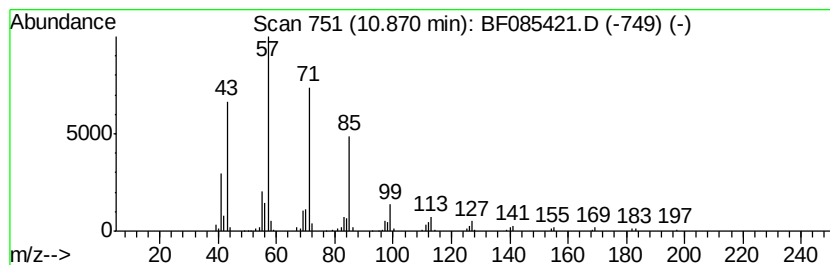
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.87	4.00 ng	326771	Phenanthrene-d10		11.45
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Tetradecane	198	C14H30	000629-59-4	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Hexadecane	226	C16H34	000544-76-3	90



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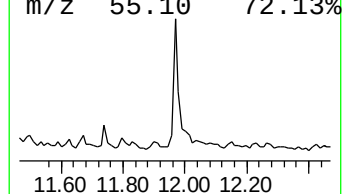
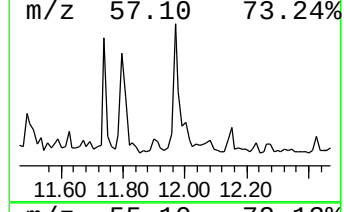
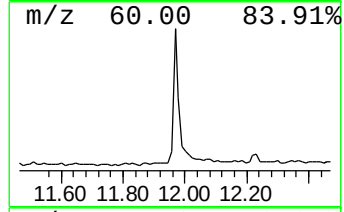
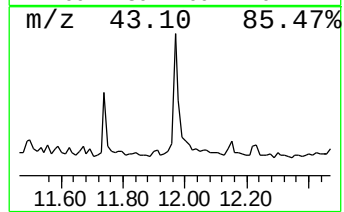
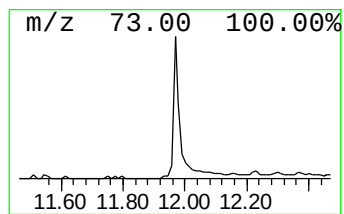
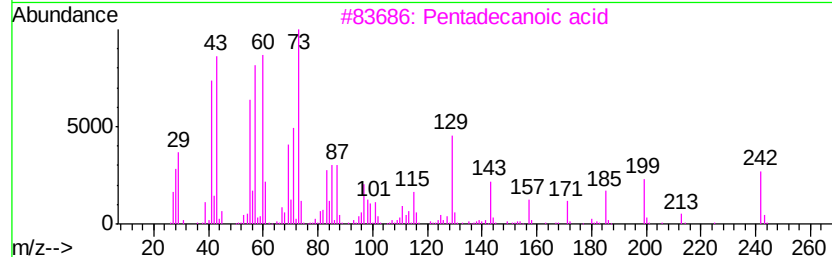
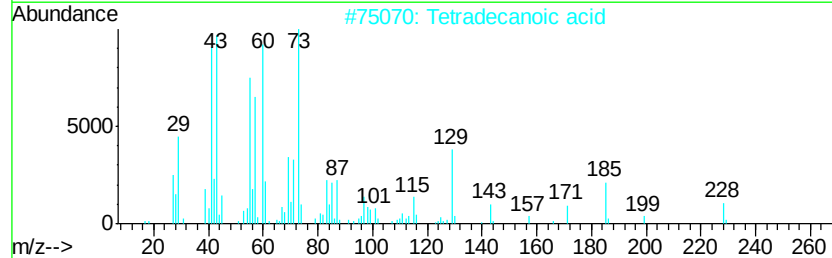
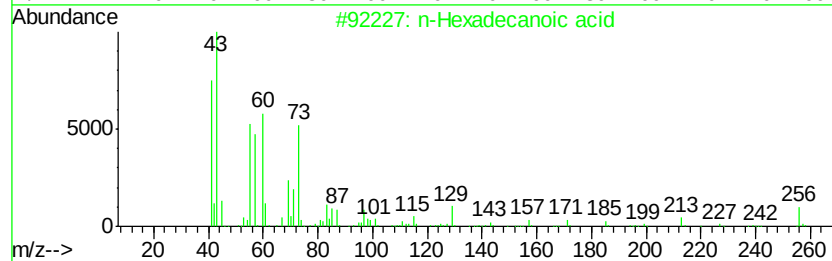
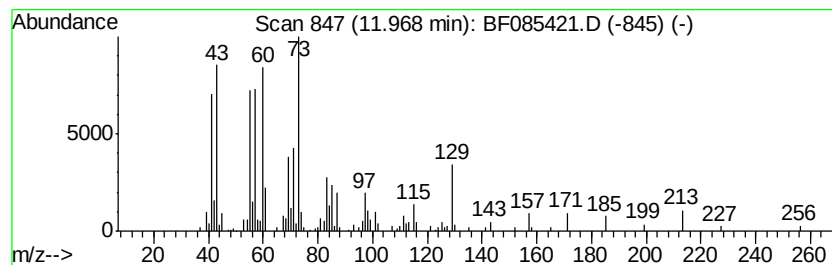
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.97	2.75 ng	224606	Phenanthrene-d10	11.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4		Dodecane	170	C12H26	000112-40-3	11
5		Undecane	156	C11H24	001120-21-4	11



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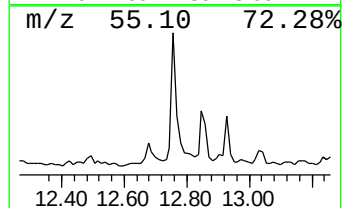
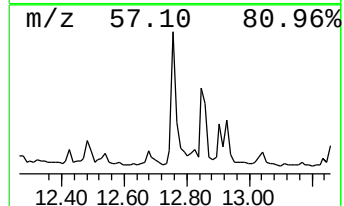
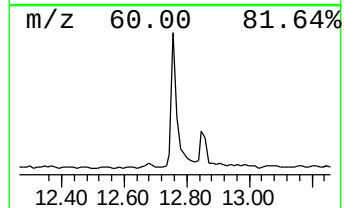
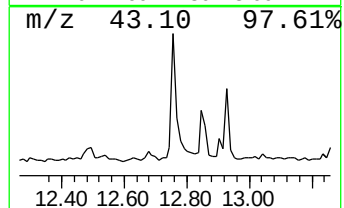
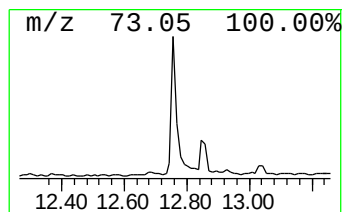
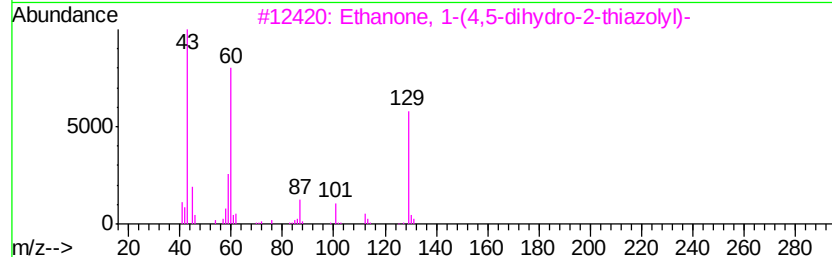
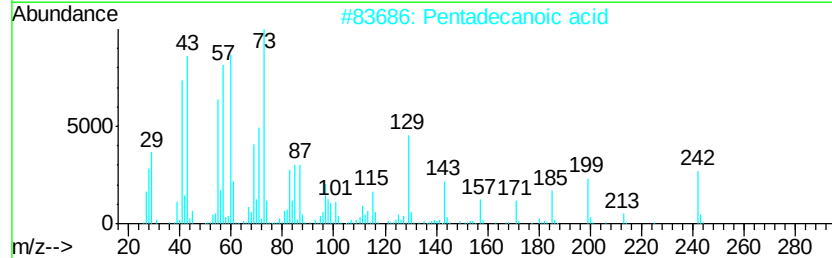
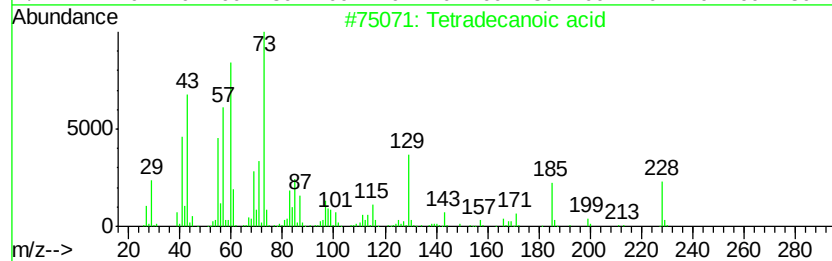
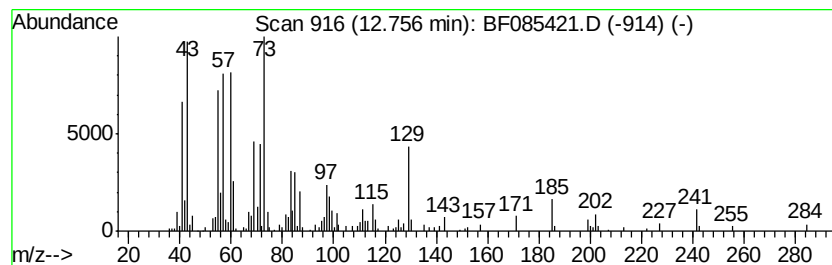
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ClientSampleId :
SB-26-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetradecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.76	3.72 ng	303564	Phenanthrene-d10		11.45
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	43
4	Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	18
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031416\
Data File : BF085421.D
Acq On : 14 Mar 2016 11:37
Operator : UM/SJ
Sample : H1731-24
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-26-COMP

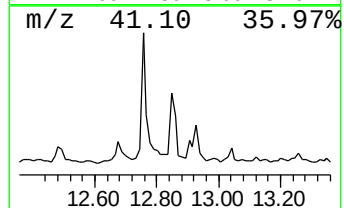
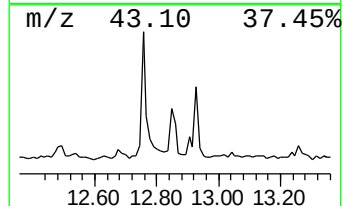
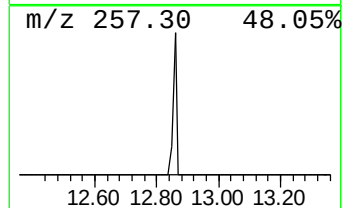
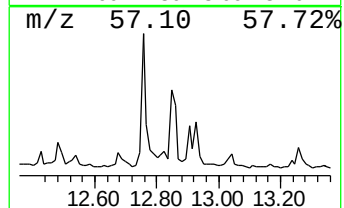
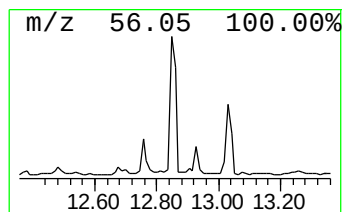
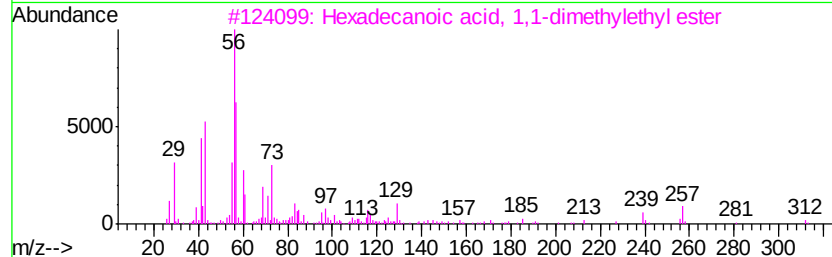
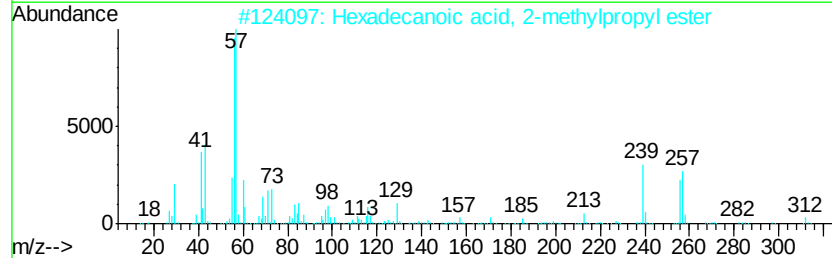
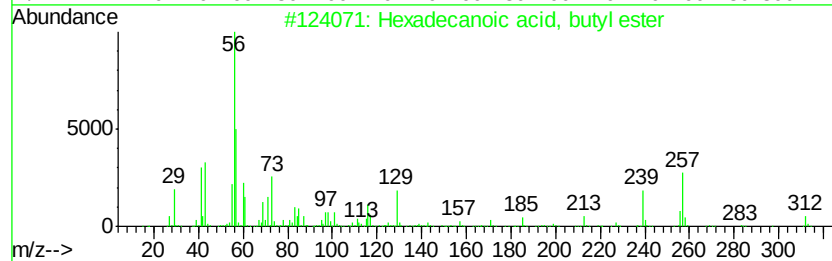
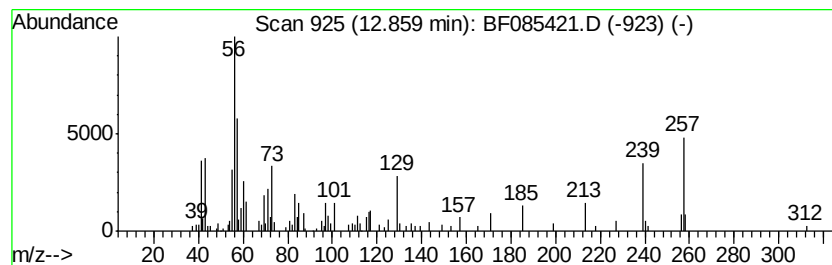
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.86	3.13 ng	149914	Chrysene-d12	14.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	89
3		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	60
4		Nipecotic acid	129	C6H11NO2	000498-95-3	38
5		1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031416\
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Sample : H1731-24
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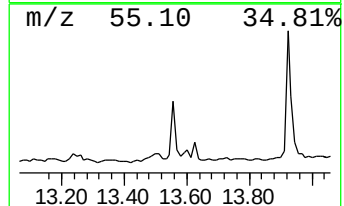
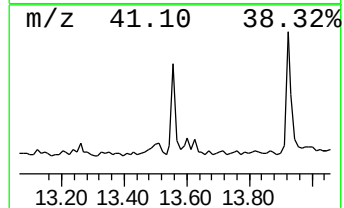
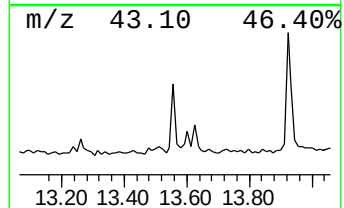
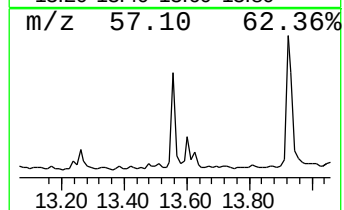
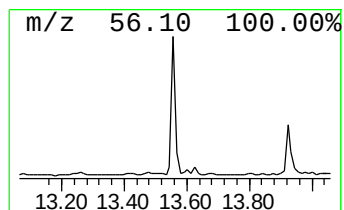
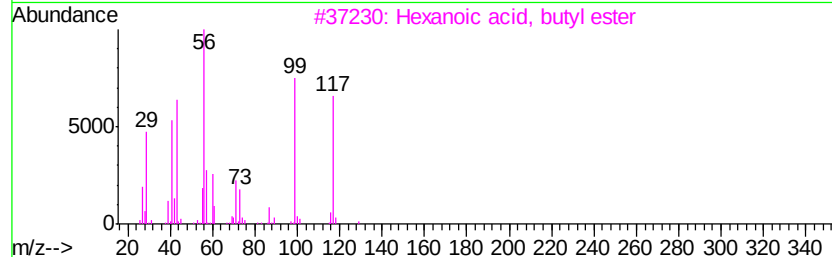
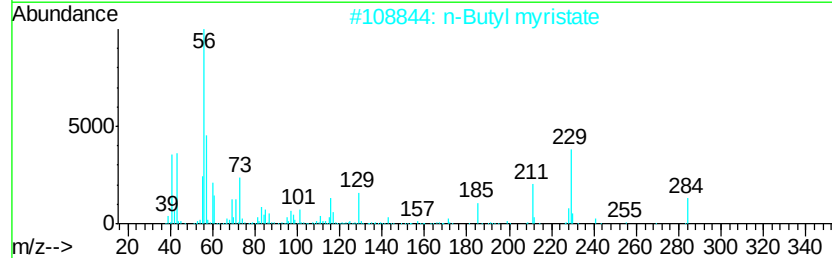
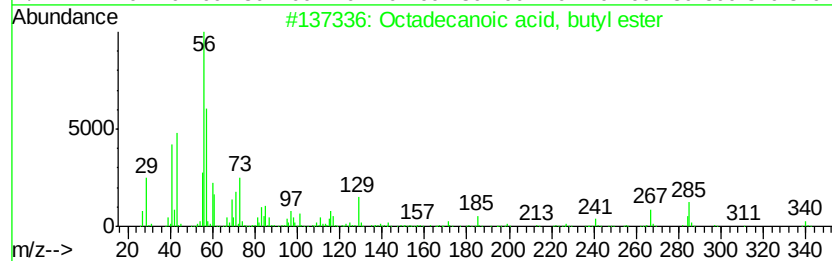
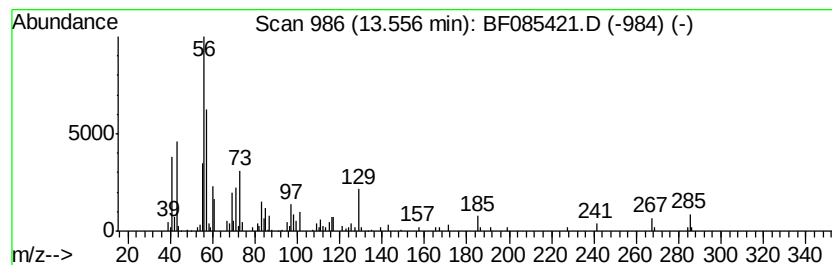
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid, butyl ester Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.56	2.31 ng	110828	Chrysene-d12		14.08	
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		Hexanoic acid, butyl ester	172	C10H20O2	000626-82-4	42
4		1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	37
5		Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031416\
Data File : BF085421.D
Acq On : 14 Mar 2016 11:37
Operator : UM/SJ
Sample : H1731-24
Misc :
ALS Vial : 3 Sample Multiplier: 1

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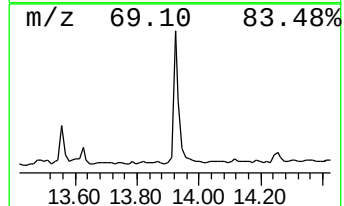
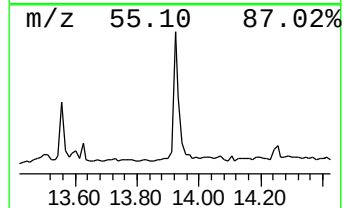
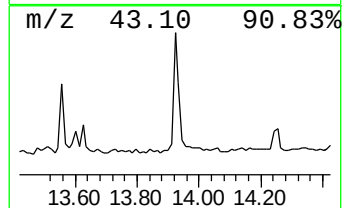
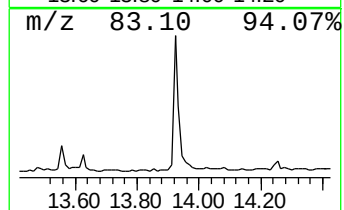
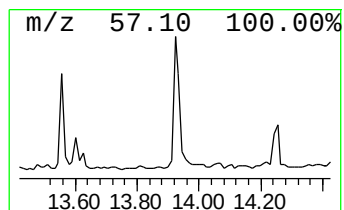
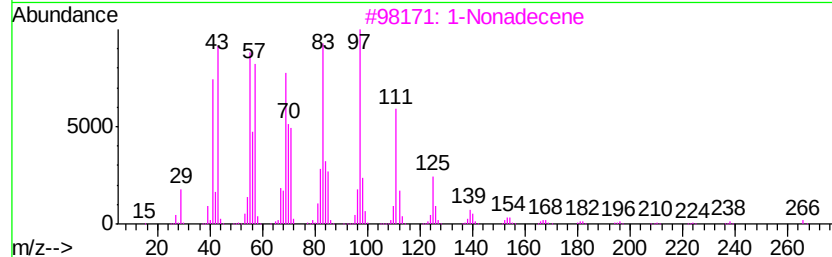
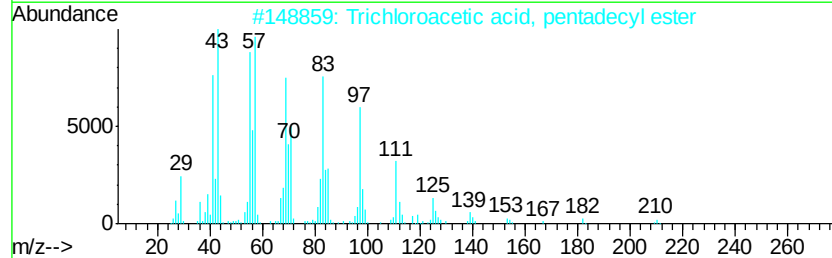
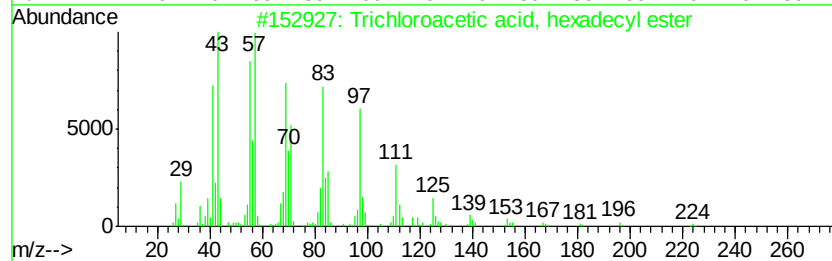
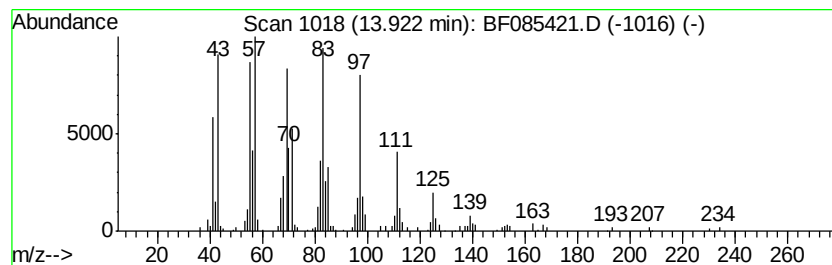
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	4.99 ng	239004	Chrysene-d12	14.08

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
3			1-Nonadecene	266	C19H38	018435-45-5	91
4			3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5			1-Octadecanol	270	C18H38O	000112-92-5	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031416\
Data File : BF085421.D
Acq On : 14 Mar 2016 11:37
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Misc :
ALS Vial : 3 Sample Multiplier: 1

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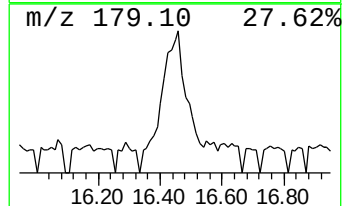
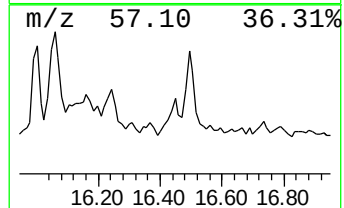
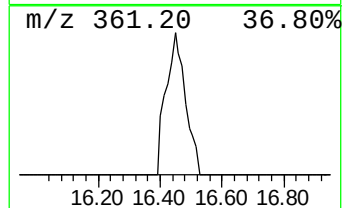
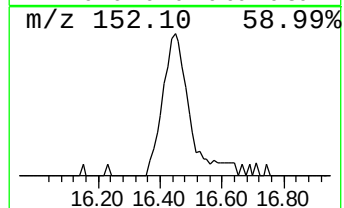
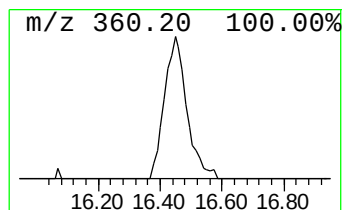
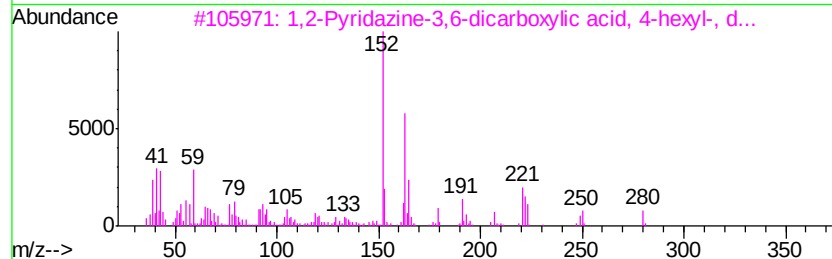
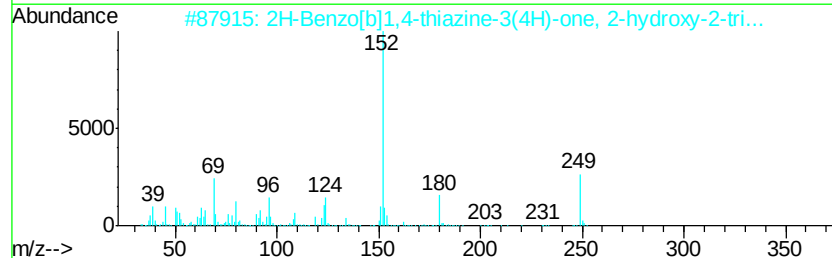
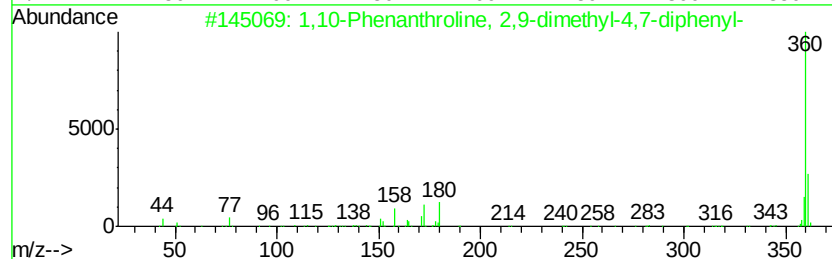
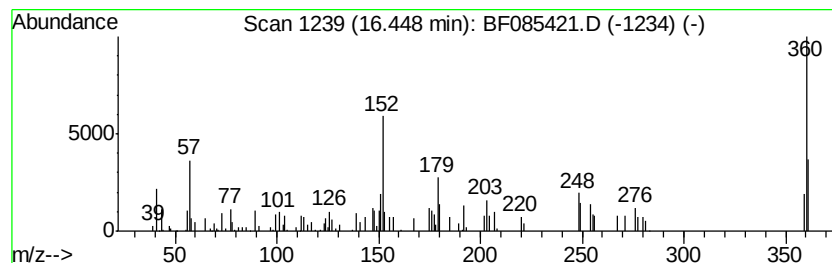
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown16.45 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.45	2.16 ng	109123	Perylene-d12	15.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	38
2		2H-Benzo[b]1,4-thiazine-3(4H)-on...	249	C9H6F3N02S	106240-09-9	10
3		1,2-Pyridazine-3,6-dicarboxylic ...	280	C14H20N2O4	1000221-47-9	9
4		1,3-Dithiane, 4,5-dimethyl-2-(4-...	254	C13H18OS2	1000197-88-6	9
5		9-Phenanthrenol, 7-ethyl-1,2,3,4...	276	C19H32O	1000146-66-1	7



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031416\
Data File : BF085421.D
Acq On : 14 Mar 2016 11:37
Operator : UM/SJ
Sample : H1731-24
Misc :
ALS Vial : 3 Sample Multiplier: 1

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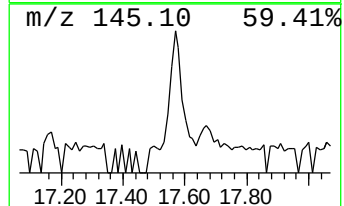
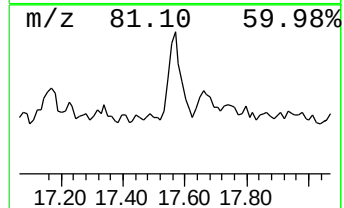
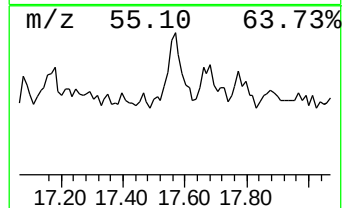
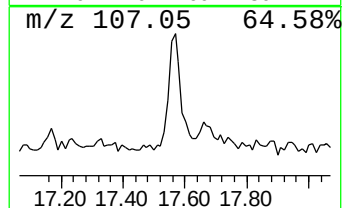
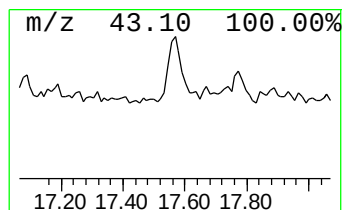
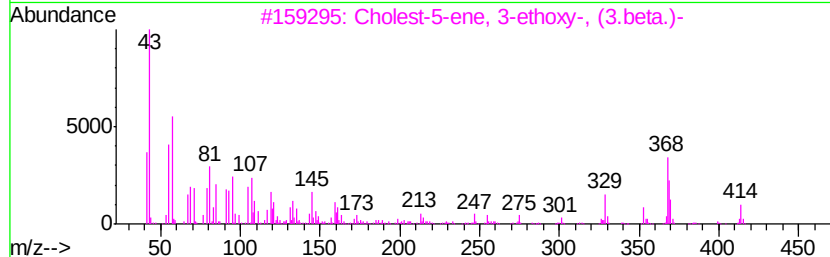
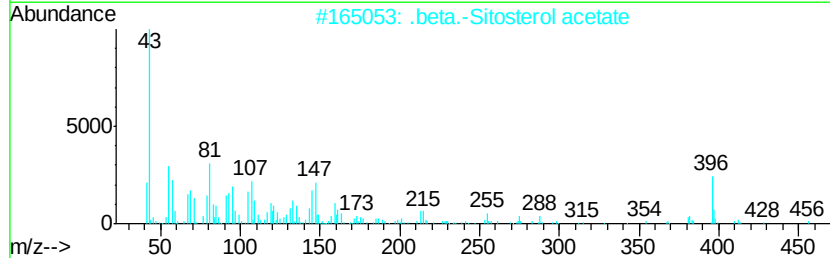
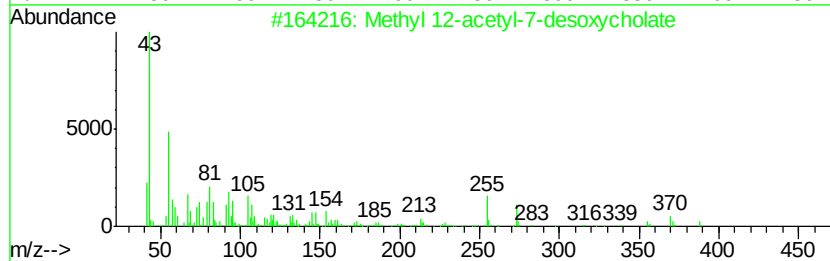
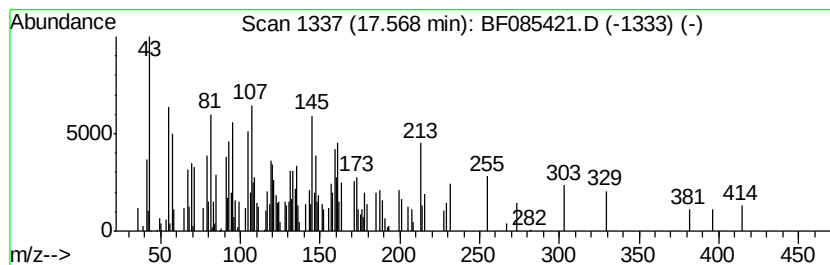
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown17.57 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.57	3.27 ng	164967	Perylene-d12	15.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methyl 12-acetyl-7-desoxycholate	448	C27H44O5	055547-48-3	35
2		.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	25
3		Cholest-5-ene, 3-ethoxy-, (3.beta...	414	C29H50O	000986-19-6	22
4		Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	12
5		Cyclohexane, 1-ethenyl-1-methyl-...	204	C15H24	000515-13-9	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031416\
Data File : BF085421.D
Acq On : 14 Mar 2016 11:37
Operator : UM/SJ
Sample : H1731-24
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.14	7.0 ng		431732	1	6.93	1239690	20.0
unknown6.70	6.70	87.6 ng		5427690	1	6.93	1239690	20.0
Tridecane	10.39	2.7 ng		232435	3	9.97	1698300	20.0
Pentadecane	10.87	4.0 ng		326771	4	11.45	1633180	20.0
n-Hexadecanoic acid	11.97	2.8 ng		224606	4	11.45	1633180	20.0
Tetradecanoic acid	12.76	3.7 ng		303564	4	11.45	1633180	20.0
Hexadecanoic acid...	12.86	3.1 ng		149914	5	14.08	958540	20.0
Octadecanoic acid...	13.56	2.3 ng		110828	5	14.08	958540	20.0
Trichloroacetic a...	13.92	5.0 ng		239004	5	14.08	958540	20.0
unknown16.45	16.45	2.2 ng		109123	6	15.55	1010410	20.0
unknown17.57	17.57	3.3 ng		164967	6	15.55	1010410	20.0