

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121217\
 Data File : BF101336.D
 Acq On : 12 Dec 2017 18:11
 Operator : SJ/JU
 Sample : I6822-02
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-1(13-15)

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-BF113017.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	5.045	500	503	514	rBV	52661	78751	5.86%	0.684%
2	5.445	567	571	587	rBV	1107264	1093710	81.35%	9.499%
3	6.463	739	744	755	rBV	1102073	1151930	85.68%	10.005%
4	6.598	762	767	770	rBV	1295941	1170861	87.08%	10.169%
5	6.822	802	805	812	rBB	328715	258877	19.25%	2.248%
6	6.981	828	832	835	rBV	997839	887991	66.05%	7.712%
7	7.392	897	902	914	rBV	695525	689137	51.26%	5.985%
8	8.104	1020	1023	1029	rBV	402646	331212	24.63%	2.877%
9	9.181	1201	1206	1209	rBV	1597934	1344509	100.00%	11.677%
10	9.251	1215	1218	1221	rBV	20674	16262	1.21%	0.141%
11	9.575	1269	1273	1279	rVB	151820	130578	9.71%	1.134%
12	9.780	1304	1308	1312	rVB	42205	30832	2.29%	0.268%
13	9.863	1318	1322	1326	rBV	420207	352015	26.18%	3.057%
14	10.280	1390	1393	1396	rVB	46342	34091	2.54%	0.296%
15	10.498	1423	1430	1433	rBV	15517	20088	1.49%	0.174%
16	10.657	1453	1457	1464	rBV	799029	715953	53.25%	6.218%
17	10.751	1471	1473	1483	rVB	40582	49992	3.72%	0.434%
18	11.204	1546	1550	1552	rBV	23086	18772	1.40%	0.163%
19	11.357	1572	1576	1578	rBV	364323	341851	25.43%	2.969%
20	11.374	1578	1579	1584	rVB	55214	42395	3.15%	0.368%
21	11.869	1656	1663	1665	rBV2	15116	23858	1.77%	0.207%
22	12.569	1779	1782	1788	rBV	105525	94648	7.04%	0.822%
23	12.739	1806	1811	1816	rBV	71308	59079	4.39%	0.513%
24	12.804	1819	1822	1825	rVB	95034	83182	6.19%	0.722%
25	12.939	1841	1845	1849	rVB	1173306	1087115	80.86%	9.442%
26	13.133	1871	1878	1880	rBV	17701	23419	1.74%	0.203%
27	13.157	1880	1882	1886	rVB	21307	16808	1.25%	0.146%
28	13.498	1936	1940	1943	rBV	42952	38410	2.86%	0.334%
29	13.827	1990	1996	1999	rBV2	132590	143744	10.69%	1.248%
30	13.963	2016	2019	2022	rBV	74580	65222	4.85%	0.566%
31	14.004	2022	2026	2029	rVV2	343165	347077	25.81%	3.014%
32	14.027	2029	2030	2034	rVB	45270	37109	2.76%	0.322%
33	14.145	2046	2050	2054	rBV	66434	63115	4.69%	0.548%
34	14.445	2099	2101	2104	rBV	53861	51498	3.83%	0.447%

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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

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35	14.751	2150	2153	2157	rVB	54935	52733	3.92%	0.458%
36	14.827	2164	2166	2171	rVB3	21152	21833	1.62%	0.190%
37	15.051	2200	2204	2206	rBV	36636	47984	3.57%	0.417%
38	15.086	2207	2210	2213	rVB2	46101	57450	4.27%	0.499%
39	15.351	2252	2255	2262	rBV	24352	32462	2.41%	0.282%
40	15.415	2263	2266	2270	rVB	35075	41589	3.09%	0.361%
41	15.480	2270	2277	2281	rBV	185104	269172	20.02%	2.338%
42	15.892	2343	2347	2351	rVB4	21429	32648	2.43%	0.284%
43	16.968	2526	2530	2536	rVB3	19200	38501	2.86%	0.334%
44	17.421	2602	2607	2612	rVB5	12582	25391	1.89%	0.221%

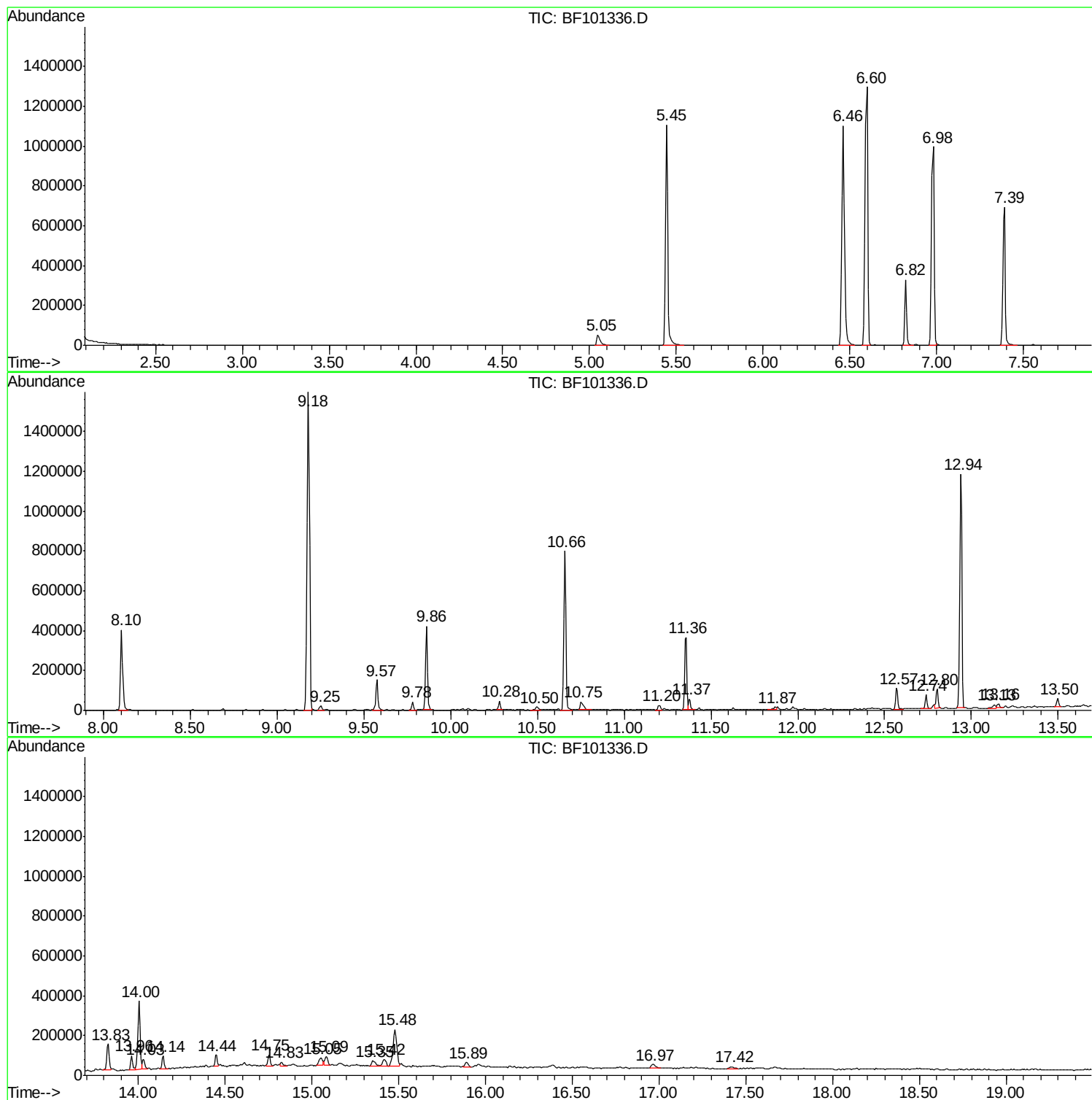
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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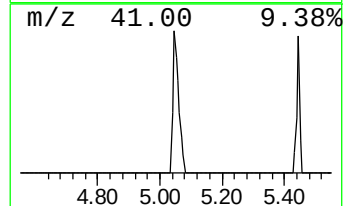
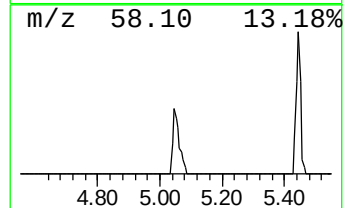
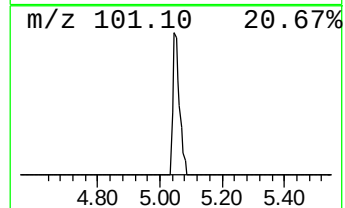
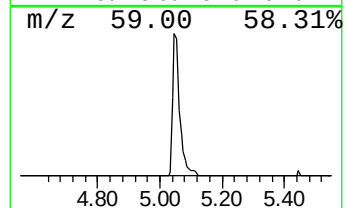
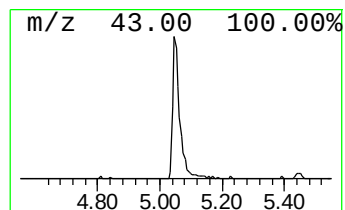
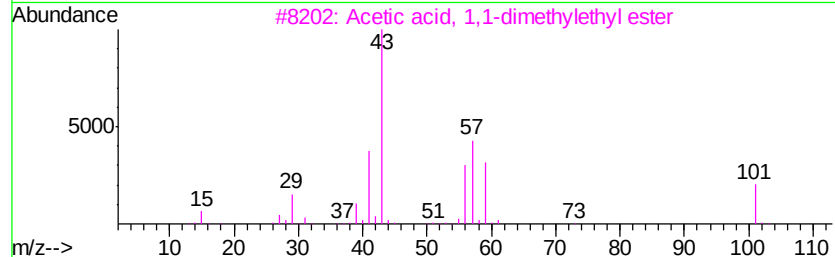
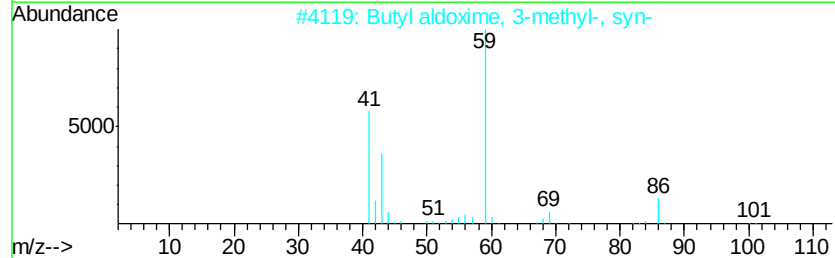
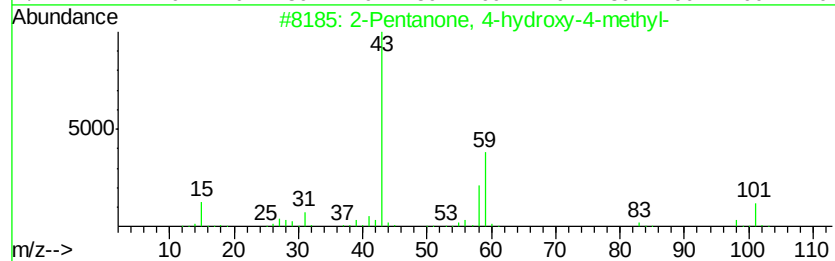
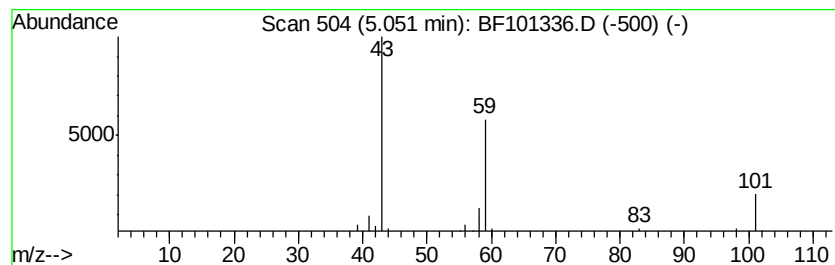
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	6.08 ng	78751	1,4-Dichlorobenzene-d4	6.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
4			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	9
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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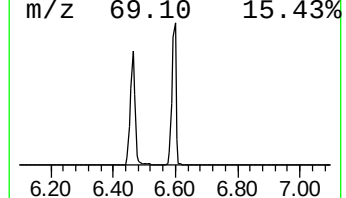
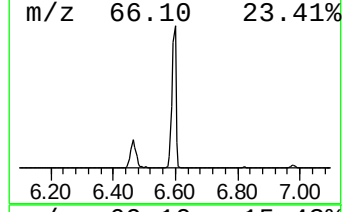
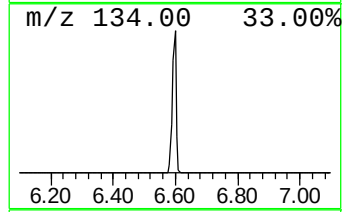
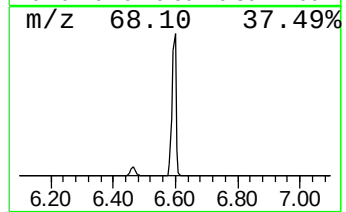
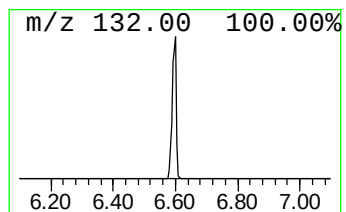
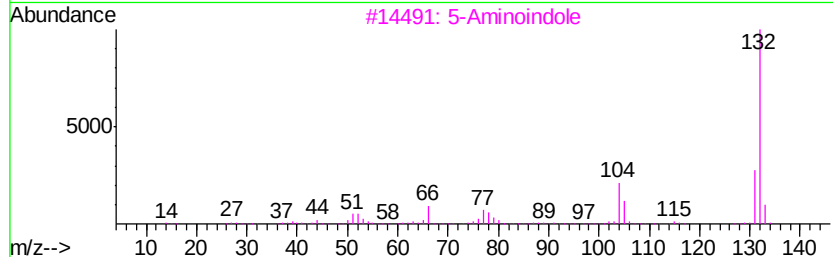
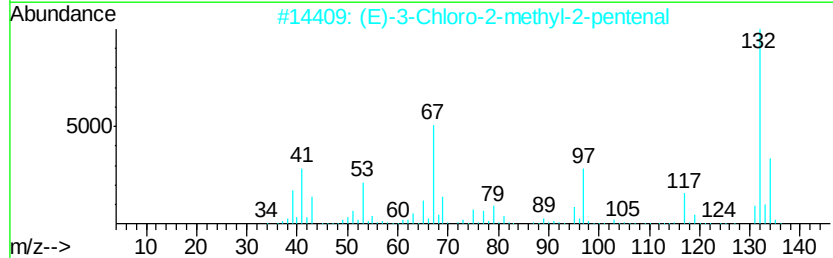
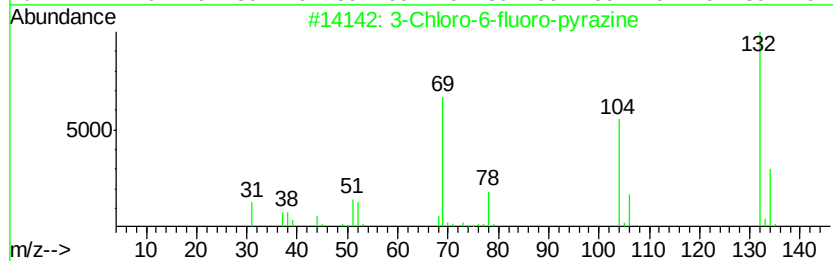
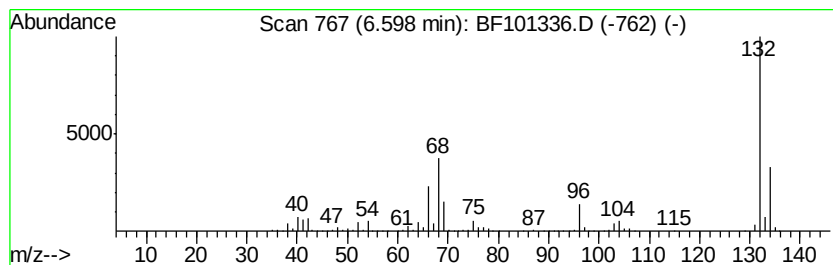
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Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	90.46 ng	1170860	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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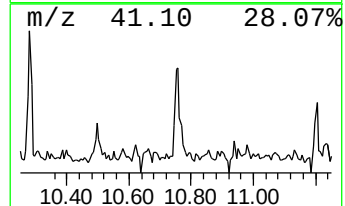
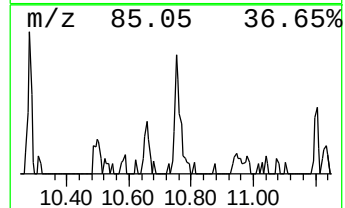
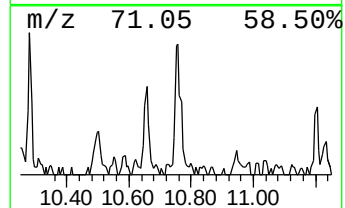
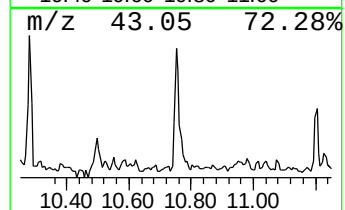
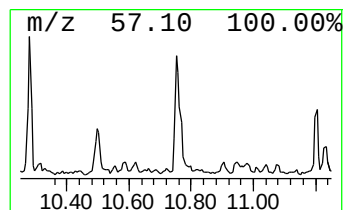
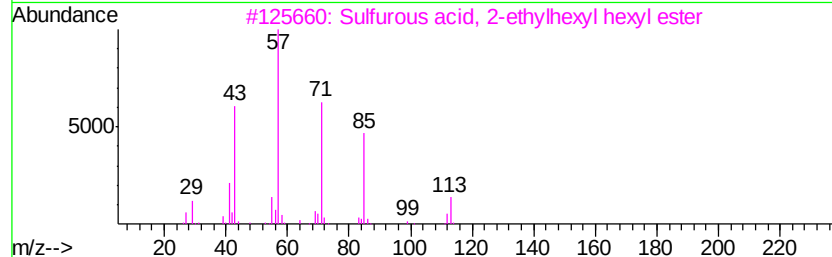
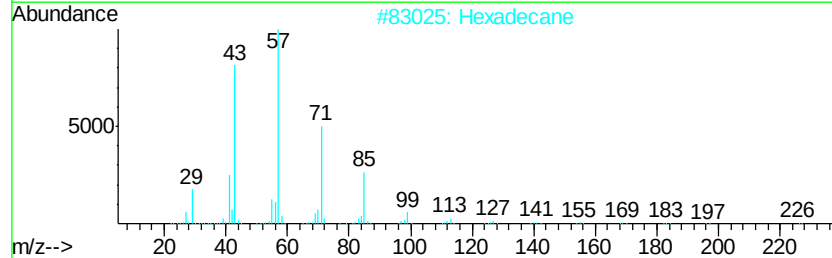
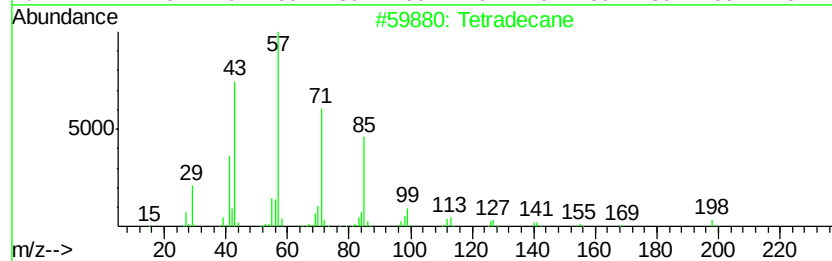
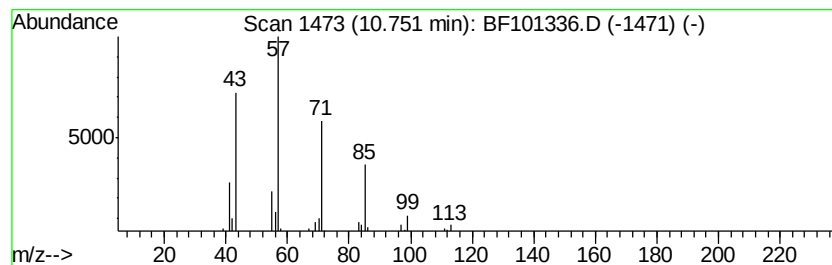
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tetradecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	2.92 ng	49992	Phenanthrene-d10	11.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Tetradecane	198 C14H30	000629-59-4 80
2		Hexadecane	226 C16H34	000544-76-3 64
3		Sulfurous acid, 2-ethylhexyl hex...	278 C14H30O3S	1000309-20-2 64
4		Heptadecane, 2,6-dimethyl-	268 C19H40	054105-67-8 59
5		2,2-Dimethyl-3-octanone	156 C10H20O	005340-64-7 50



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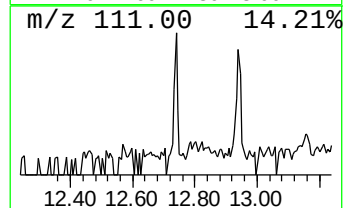
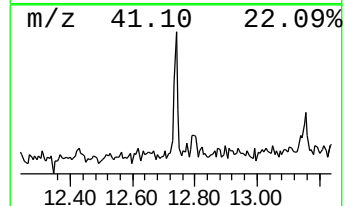
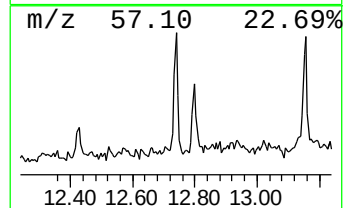
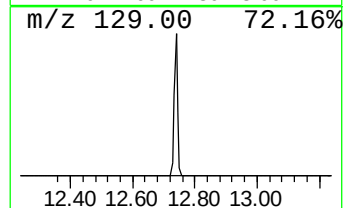
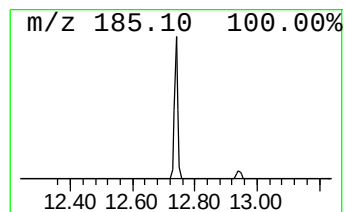
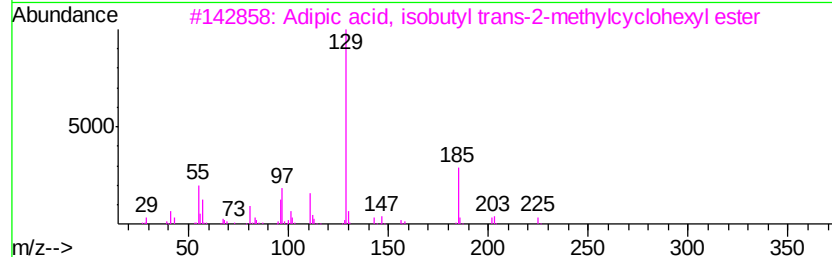
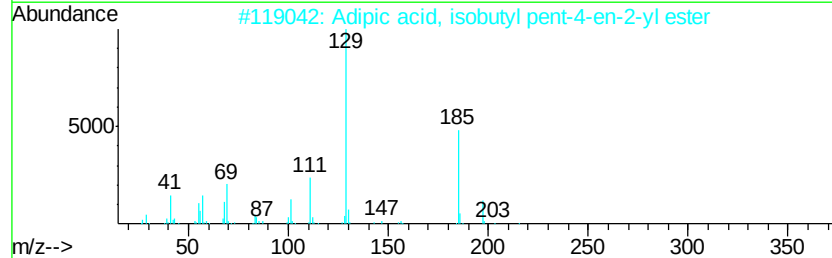
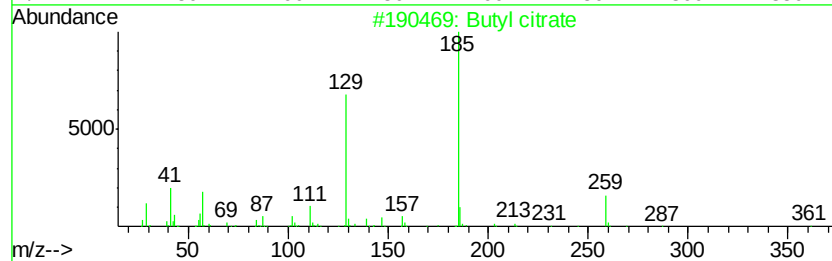
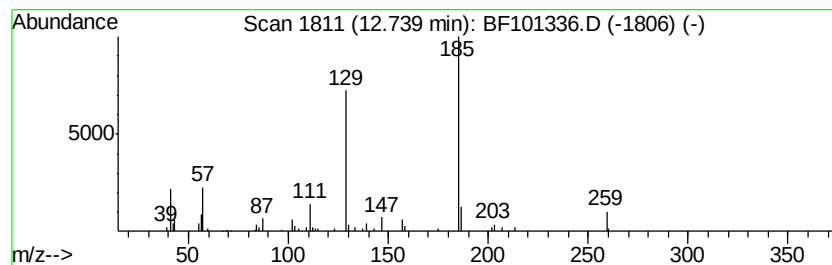
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Butyl citrate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	3.40 ng	59079	Chrysene-d12	14.00
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Butyl citrate	360 C18H32O7	000077-94-1	91
2	Adipic acid, isobutyl pent-4-en-...	270 C15H26O4	1000354-11-8	64
3	Adipic acid, isobutyl trans-2-me...	298 C17H30O4	1000324-74-5	56
4	Hexanedioic acid, bis(2-methylpr...	258 C14H26O4	000141-04-8	50
5	Adipic acid, butyl 2,4-dimethylp...	300 C17H32O4	1000349-77-7	50



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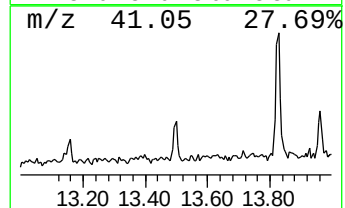
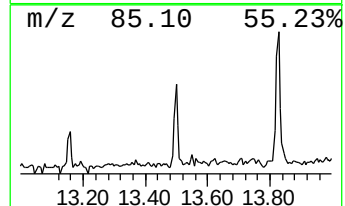
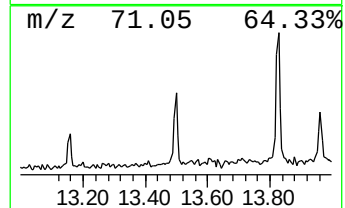
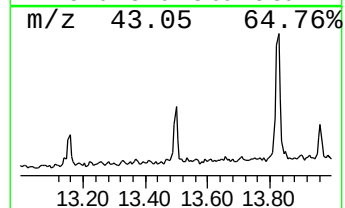
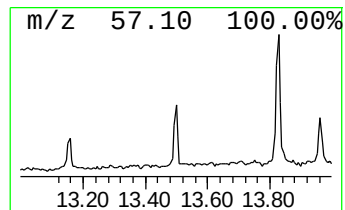
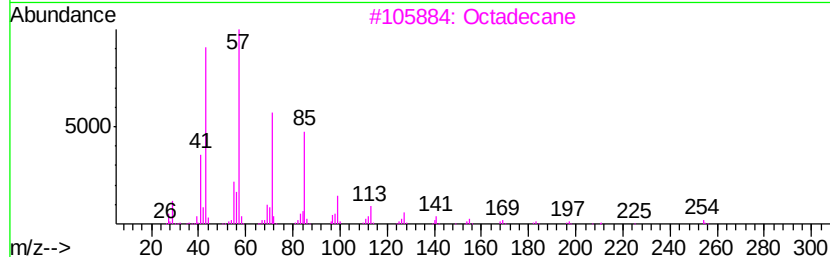
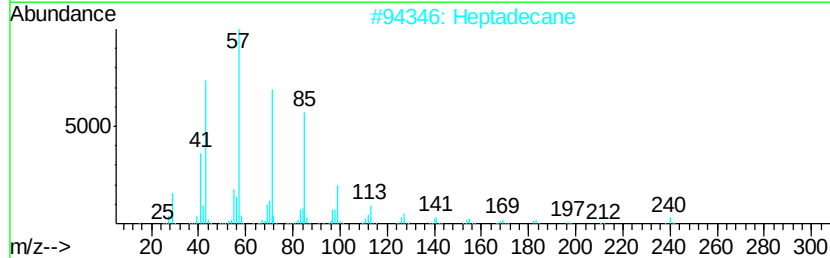
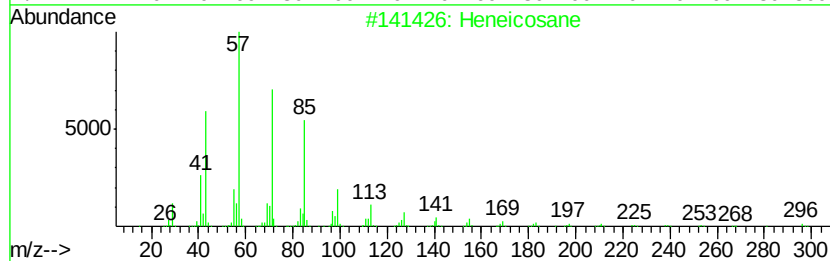
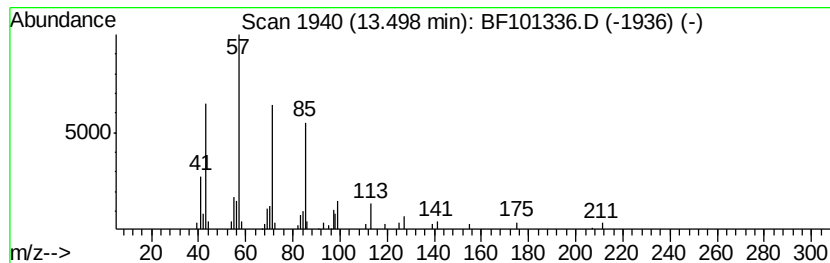
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Heneicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.50	2.21 ng	38410	Chrysene-d12	14.00	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	87
2	Heptadecane	240	C17H36	000629-78-7	87
3	Octadecane	254	C18H38	000593-45-3	86
4	Hexadecane	226	C16H34	000544-76-3	86
5	Triacontane	422	C30H62	000638-68-6	80



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121217\
Data File : BF101336.D
Acq On : 12 Dec 2017 18:11
Operator : SJ/JU
Sample : I6822-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-1(13-15)

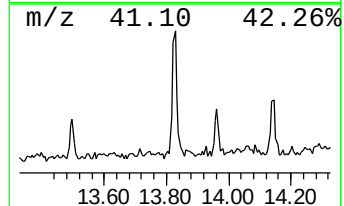
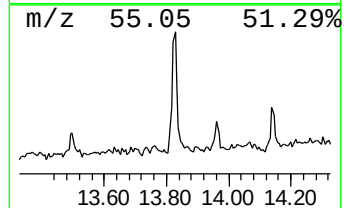
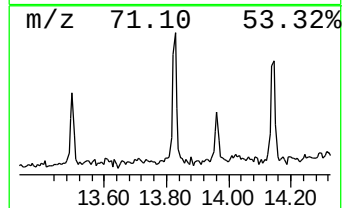
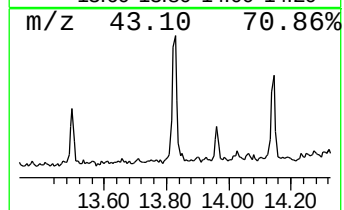
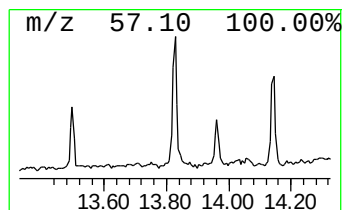
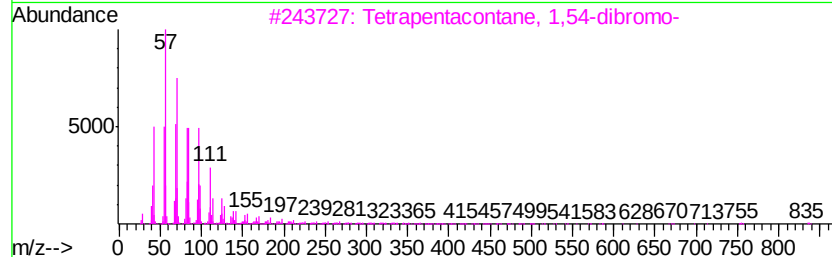
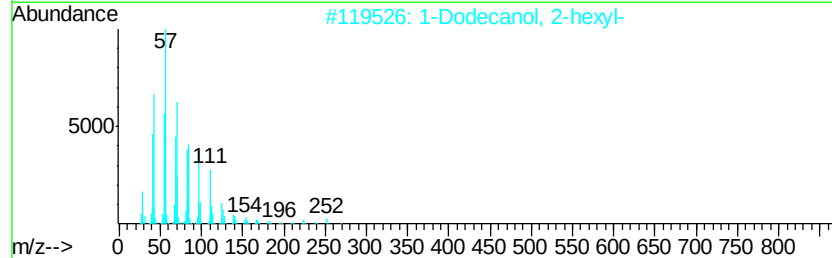
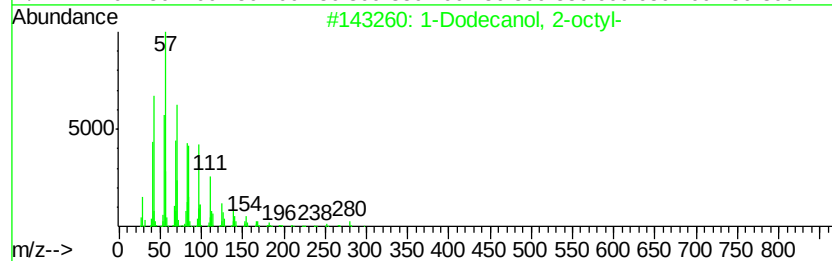
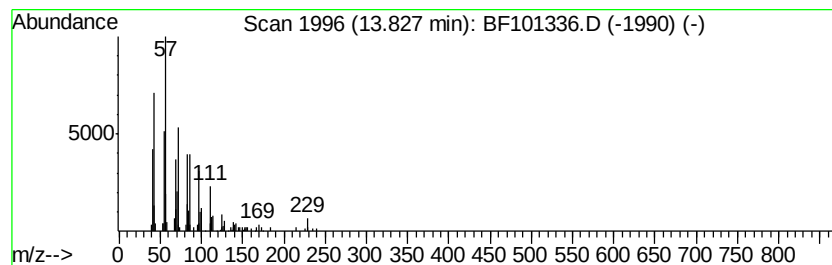
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Dodecanol, 2-octyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	8.28 ng	143744	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
2		1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	87
3		Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	68
4		1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	64
5		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	62



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121217\
Data File : BF101336.D
Acq On : 12 Dec 2017 18:11
Operator : SJ/JU
Sample : I6822-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

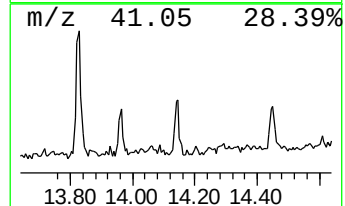
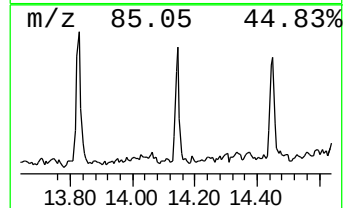
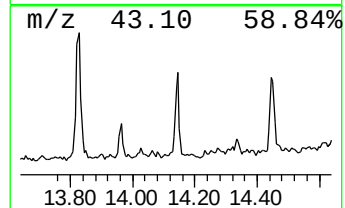
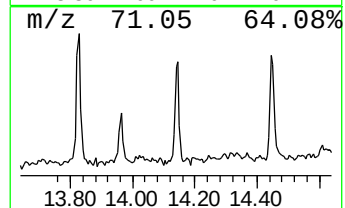
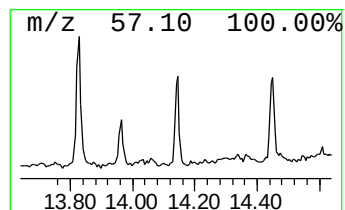
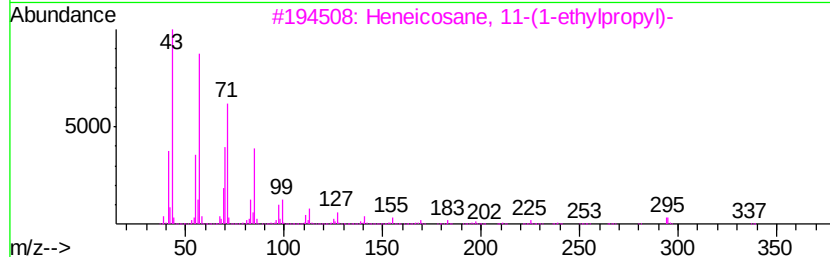
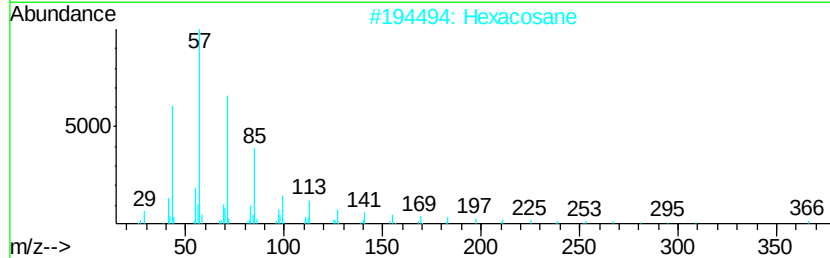
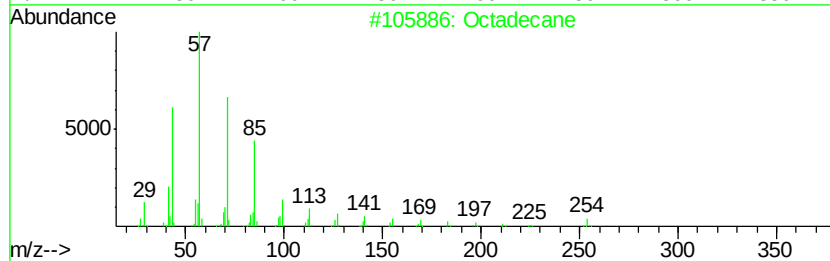
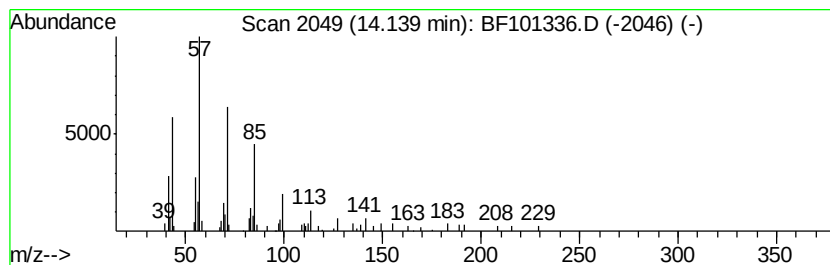
Instrument :
BNA_F
ClientSampleId :
SB-1(13-15)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.14	3.64 ng	63115	Chrysene-d12		14.00
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	87
2	Hexacosane	366	C26H54	000630-01-3	87
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
4	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	86
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121217\
Data File : BF101336.D
Acq On : 12 Dec 2017 18:11
Operator : SJ/JU
Sample : I6822-02
Misc :
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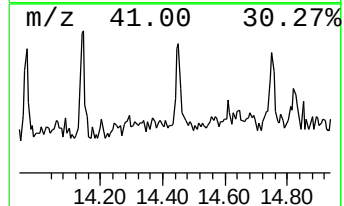
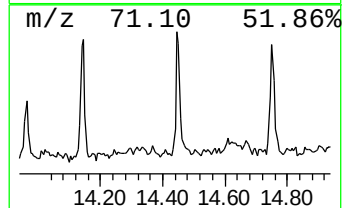
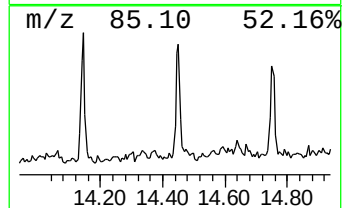
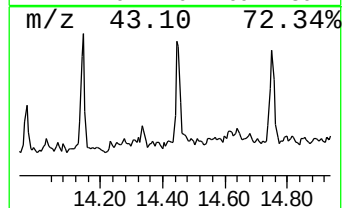
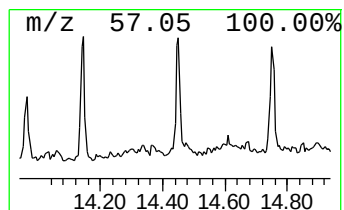
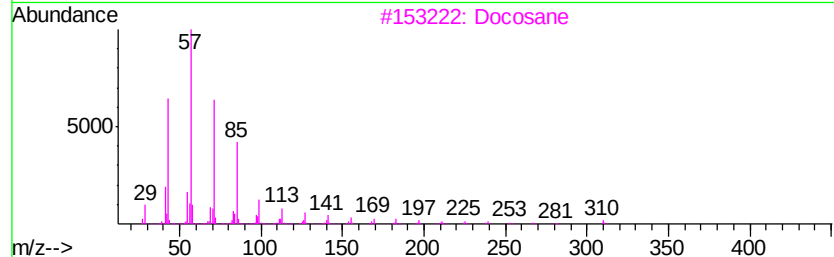
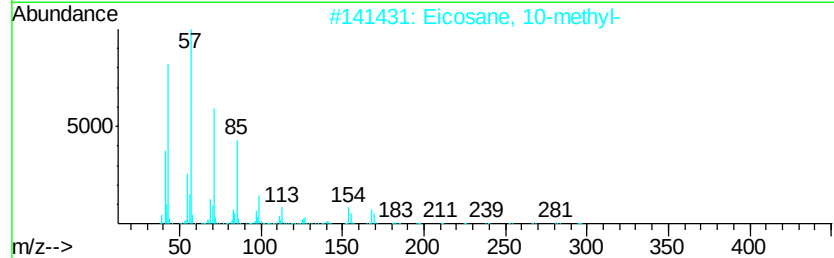
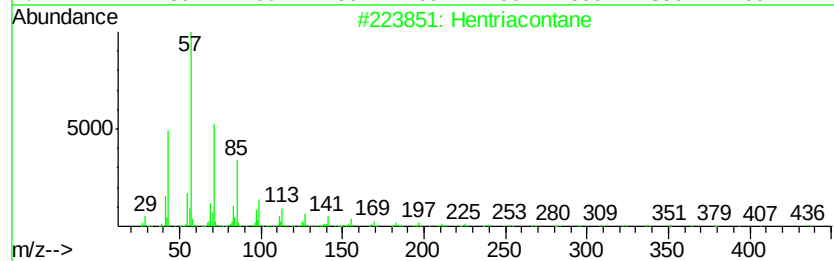
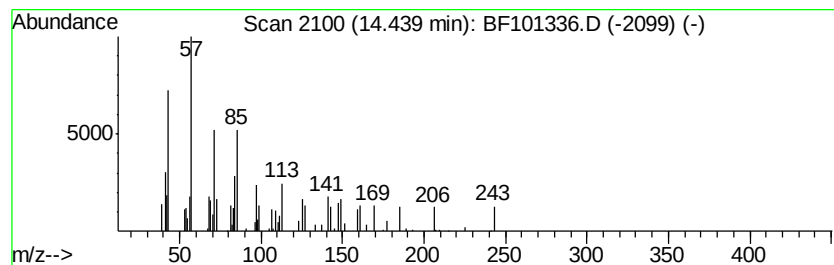
Instrument :
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ClientSampleId :
SB-1(13-15)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hentriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.44	2.97 ng	51498	Chrysene-d12	14.00
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hentriacontane	437 C31H64	000630-04-6	90
2	Eicosane, 10-methyl-	296 C21H44	054833-23-7	87
3	Docosane	310 C22H46	000629-97-0	87
4	Triacontane	422 C30H62	000638-68-6	87
5	Octadecane	254 C18H38	000593-45-3	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121217\
Data File : BF101336.D
Acq On : 12 Dec 2017 18:11
Operator : SJ/JU
Sample : I6822-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

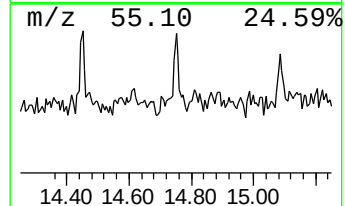
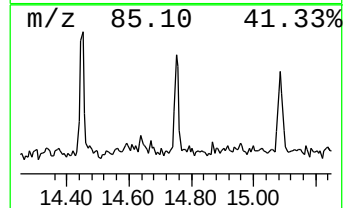
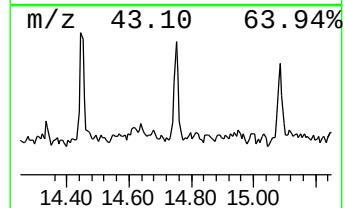
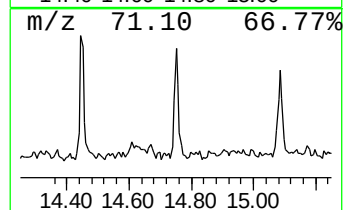
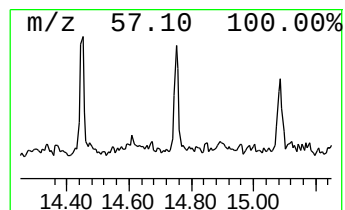
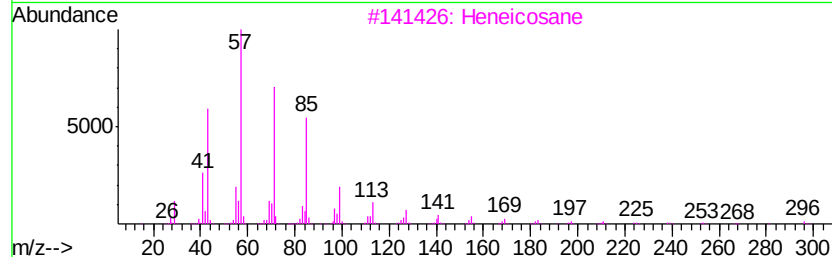
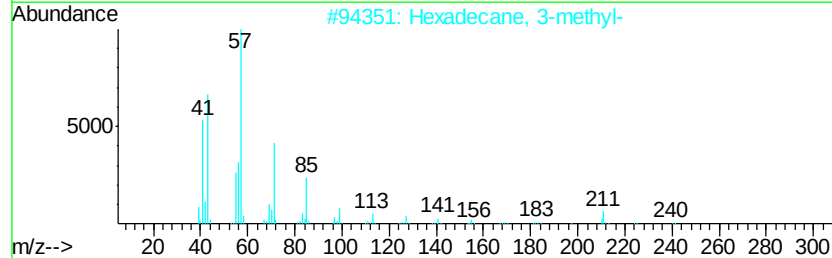
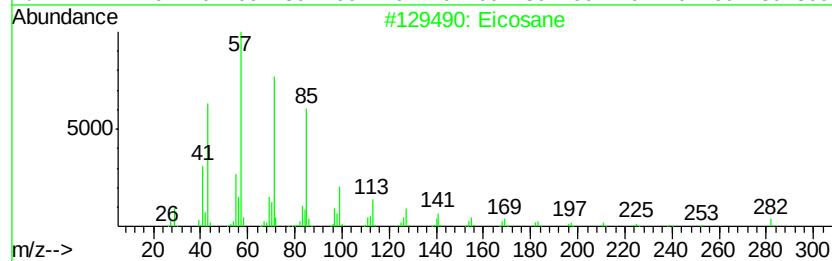
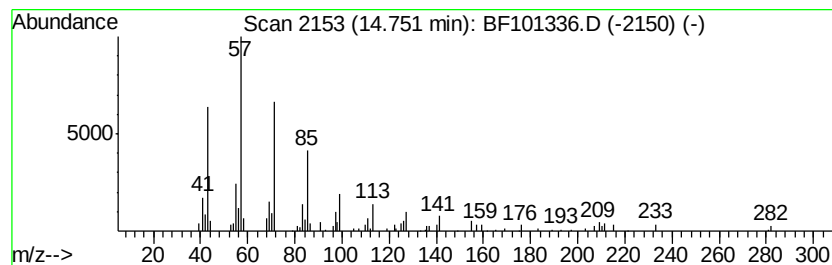
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.75	3.92 ng	52733	Perylene-d12		15.48
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Hexadecane, 3-methyl-	240	C17H36	006418-43-5	90
3	Heneicosane	296	C21H44	000629-94-7	87
4	Heptacosane	380	C27H56	000593-49-7	87
5	Pentacosane	352	C25H52	000629-99-2	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121217\
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Sample : I6822-02
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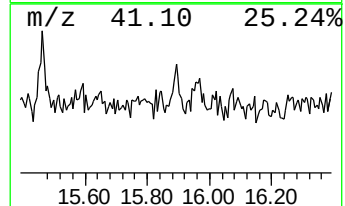
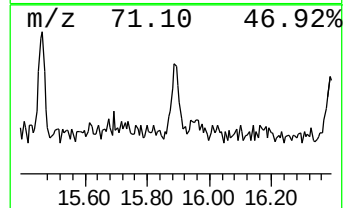
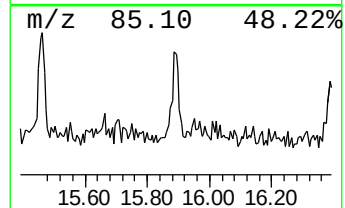
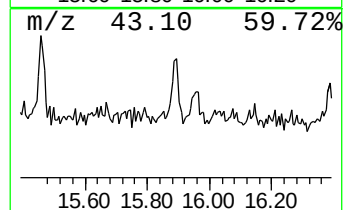
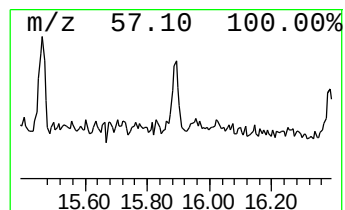
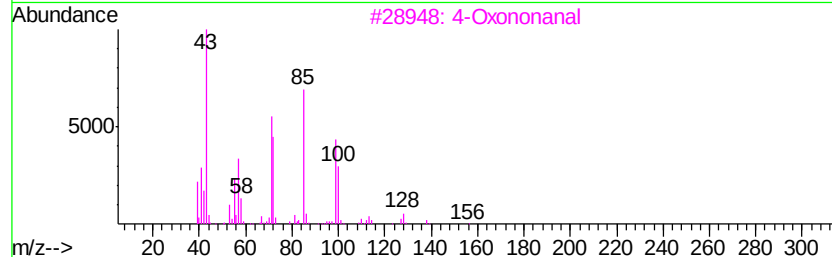
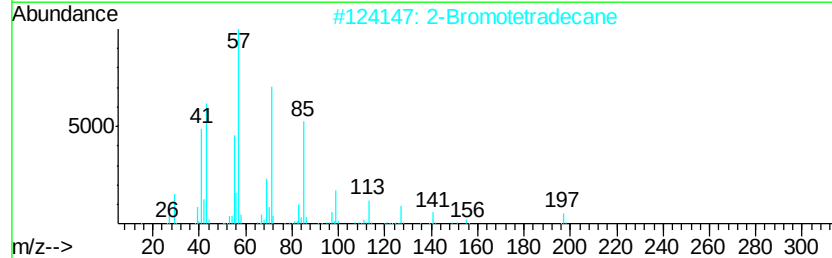
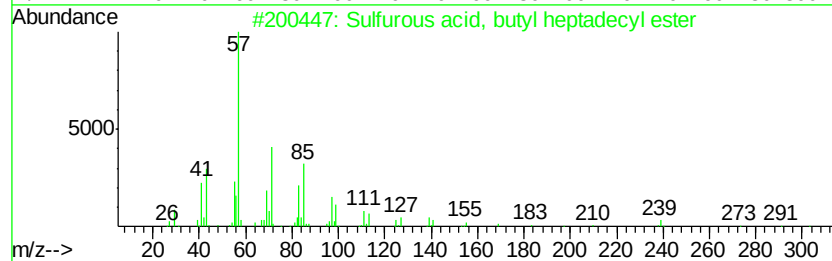
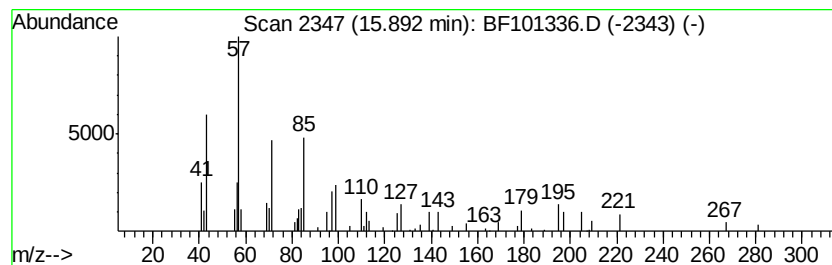
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Sulfurous acid, butyl hepta... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.89	2.43 ng	32648	Perylene-d12	15.48	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	50
2	2-Bromotetradecane	276	C14H29Br	074036-95-6	43
3	4-Oxononanal	156	C9H16O2	1000314-10-4	43
4	Nonadecane	268	C19H40	000629-92-5	38
5	Decane, 2,4,6-trimethyl-	184	C13H28	062108-27-4	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121217\
Data File : BF101336.D
Acq On : 12 Dec 2017 18:11
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Sample : I6822-02
Misc :
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Instrument :
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ClientSampleId :
SB-1(13-15)

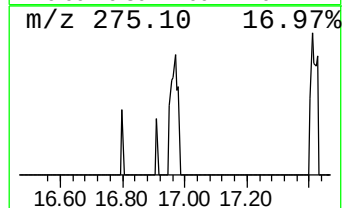
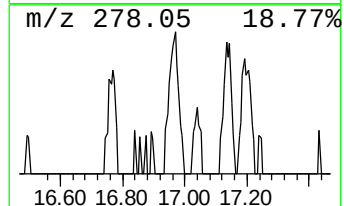
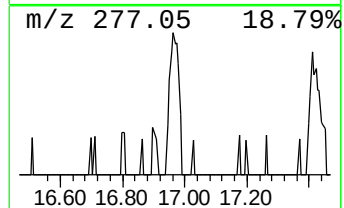
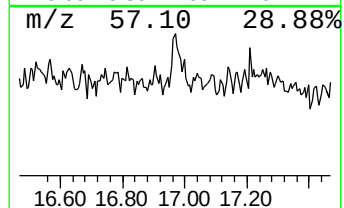
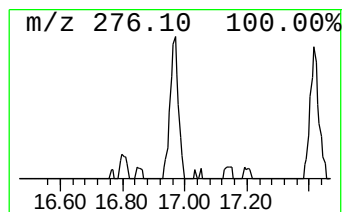
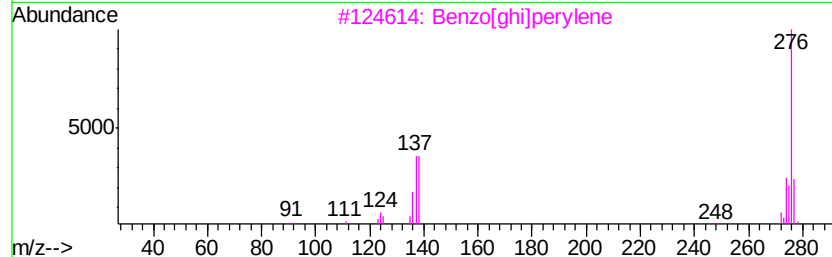
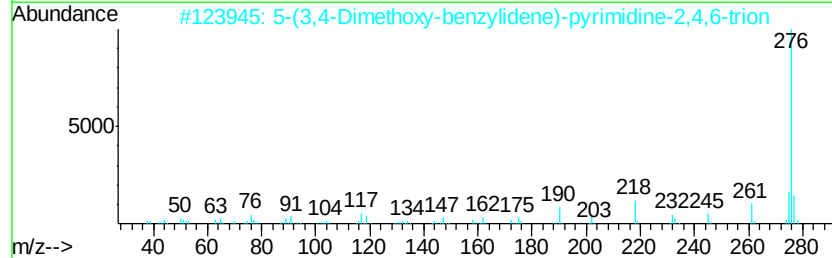
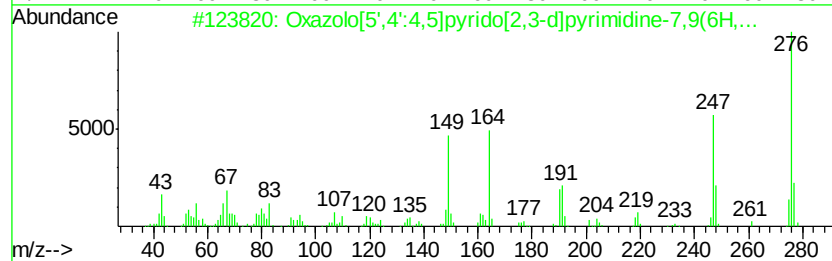
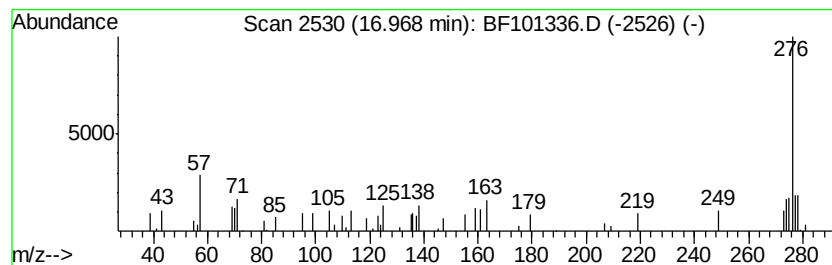
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Oxazolo[5',4':4,5]pyrido[2,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.97	2.86 ng	38501	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxazolo[5',4':4,5]pyrido[2,3-d]p...	276	C12H12N4O4	349496-92-0	53
2		5-(3,4-Dimethoxy-benzylidene)-py...	276	C13H12N2O5	1000318-16-4	50
3		Benzo[ghi]perylene	276	C22H12	000191-24-2	50
4		2-(p-Tolyl)oxazolo[4,5-c]quinoli...	276	C17H12N2O2	148563-22-8	50
5		1H-Cyclopenta[4,5]pyrido[1,2-a]b...	276	C17H16N4	329707-31-5	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121217\
Data File : BF101336.D
Acq On : 12 Dec 2017 18:11
Operator : SJ/JU
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-1(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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...	5.05	6.1 ng		78751	1	6.82	258877	20.0
unknown6.60	6.60	90.5 ng		1170860	1	6.82	258877	20.0
Tetradecane	10.75	2.9 ng		49992	4	11.35	341851	20.0
Butyl citrate	12.74	3.4 ng		59079	5	14.00	347077	20.0
Heneicosane	13.50	2.2 ng		38410	5	14.00	347077	20.0
1-Dodecanol, 2-oc...	13.83	8.3 ng		143744	5	14.00	347077	20.0
Octadecane	14.14	3.6 ng		63115	5	14.00	347077	20.0
Hentriacontane	14.44	3.0 ng		51498	5	14.00	347077	20.0
Eicosane	14.75	3.9 ng		52733	6	15.48	269172	20.0
Sulfurous acid, b...	15.89	2.4 ng		32648	6	15.48	269172	20.0
Oxazolo[5',4':4,5...	16.97	2.9 ng		38501	6	15.48	269172	20.0