LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101015\
Data File : BF082203.D
Acq On : 11 Oct 2015 4:41
Operator : UM/IZ
Sample : G3979-06
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A14COMP

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-BF101015.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	5.017	249	252	264	rVB	672397	1164960	58.35%	5.249%
2	5.440	286	289	291	rBV	1792526	1889411	94.63%	8.513%
3	6.137	347	350	360	rVB	21464	34737	1.74%	0.157%
4	6.469	376	379	382	rBV	1287119	1841227	92.22%	8.296%
5	6.606	388	391	393	rBV	2053109	1996561	100.00%	8.996%
6	6.835	409	411	414	rBV	600851	548872	27.49%	2.473%
7	6.995	422	425	427	rBV	1539303	1533314	76.80%	6.908%
8	7.406	458	461	468	rBV	1134912	1190491	59.63%	5.364%
9	7.497	468	469	475	rVB	12572	23428	1.17%	0.106%
10	8.023	514	515	521	rBV2	41769	68457	3.43%	0.308%
11	8.126	521	524	526	rBV	711943	727673	36.45%	3.279%
12	8.366	541	545	552	rVB2	18475	36818	1.84%	0.166%
13	9.075	604	607	612	rVB	36378	44470	2.23%	0.200%
14	9.200	615	618	621	rBV	2009227	1987837	99.56%	8.956%
15	9.315	626	628	631	rVV	329684	320974	16.08%	1.446%
16	9.600	650	653	655	rBV	398612	366482	18.36%	1.651%
17	9.875	675	677	680	rBV	711958	834210	41.78%	3.759%
18	10.309	710	715	716	rBV3	29974	55707	2.79%	0.251%
19	10.458	726	728	730	rBV	192463	179330	8.98%	0.808%
20	10.675	744	747	749	rBV	1080117	1401286	70.18%	6.314%
21	10.778	755	756	761	rVB	45572	53436	2.68%	0.241%
22	10.881	763	765	767	rBV	20747	20779	1.04%	0.094%
23	11.224	793	795	797	rBV	35534	35579	1.78%	0.160%
24	11.361	805	807	810	rBV	669157	809939	40.57%	3.649%
25	11.532	820	822	824	rBV	21453	22635	1.13%	0.102%
26	11.589	825	827	831	rVV	91152	100898	5.05%	0.455%
27	11.658	831	833	834	rBV	17128	20851	1.04%	0.094%
28	11.898	852	854	856	rBV	89404	109972	5.51%	0.495%
29	12.058	866	868	870	rVV	23676	21161	1.06%	0.095%
30	12.092	870	871	874	rVV2	36384	42509	2.13%	0.192%
31	12.138	874	875	879	rVB	30179	29855	1.50%	0.135%
32	12.412	895	899	908	rBV	144271	254213	12.73%	1.145%
33	12.595	912	915	917	rBV2	25135	44089	2.21%	0.199%
34	12.641	917	919	920	rBV	40631	36603	1.83%	0.165%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
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Integration Parameters: rteint.p
Integrator: RTE
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.664	920	921	924	rVB2	159877	145336	7.28%	0.655%
36	12.767	928	930	933	rBV2	263748	332538	16.66%	1.498%
37	12.824	933	935	936	rVB	25761	26917	1.35%	0.121%
38	12.892	939	941	944	rBV	29386	35627	1.78%	0.161%
39	12.949	944	946	949	rBV	1712279	1747771	87.54%	7.875%
40	13.178	963	966	968	rBV	48190	54275	2.72%	0.245%
41	13.269	971	974	975	rBV3	19171	20934	1.05%	0.094%
42	13.407	983	986	989	rVB2	38751	45238	2.27%	0.204%
43	13.475	989	992	994	rVB	87282	79280	3.97%	0.357%
44	13.521	994	996	997	rBV	56740	52872	2.65%	0.238%
45	13.841	1022	1024	1034	rBV	191788	293681	14.71%	1.323%
46	14.001	1036	1038	1041	rVV	617134	668276	33.47%	3.011%
47	14.161	1050	1052	1058	rVB	21844	31041	1.55%	0.140%
48	14.470	1075	1079	1085	rBV2	28640	64687	3.24%	0.291%
49	14.767	1101	1105	1108	rBV2	25554	44845	2.25%	0.202%
50	14.835	1109	1111	1114	rVB	36961	45016	2.25%	0.203%
51	15.441	1161	1164	1172	rBV	444430	582042	29.15%	2.622%
52	15.875	1199	1202	1204	rBV	14063	23874	1.20%	0.108%
53	15.933	1204	1207	1210	rBV2	13295	27148	1.36%	0.122%
54	16.904	1289	1292	1297	rVB3	10253	24748	1.24%	0.112%

Sum of corrected areas: 22194910

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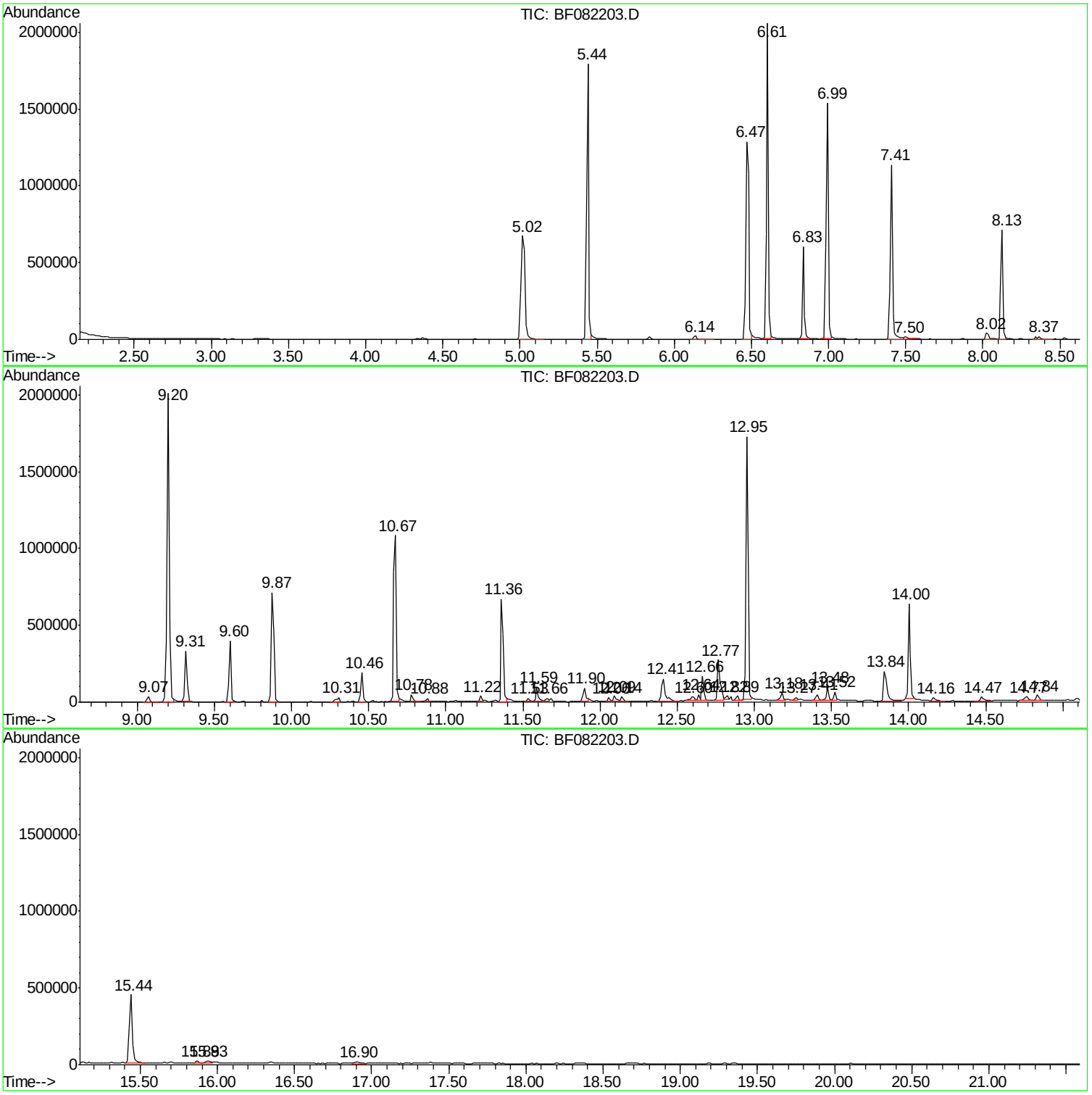
Instrument : BNA_F
ClientSampleId : A14COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Data File : BF082203.D
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Operator : UM/IZ
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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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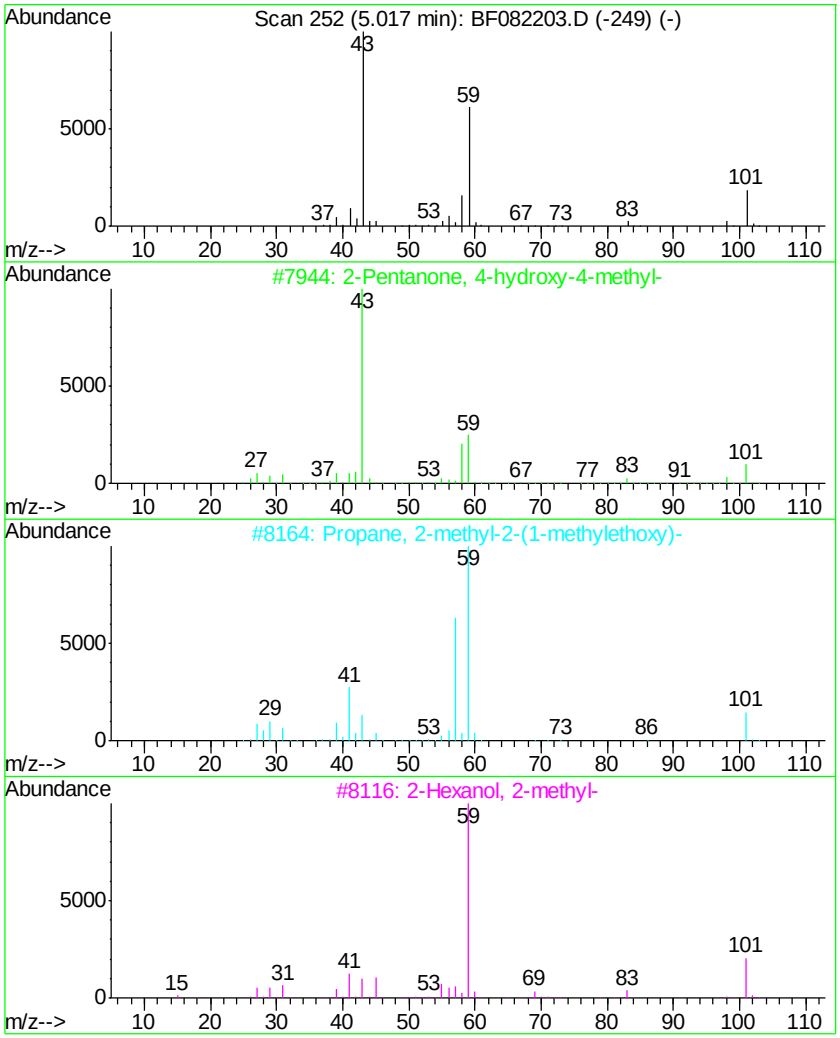
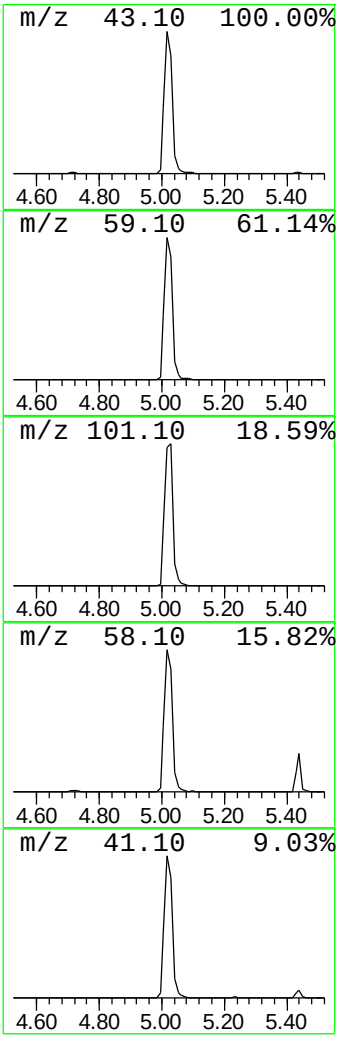
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	42.45 ng	1164960	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	40
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	t-Butyl ethyl ether	102	C6H14O	1000118-18-4	23





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Operator : UM/IZ
Sample : G3979-06
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A14COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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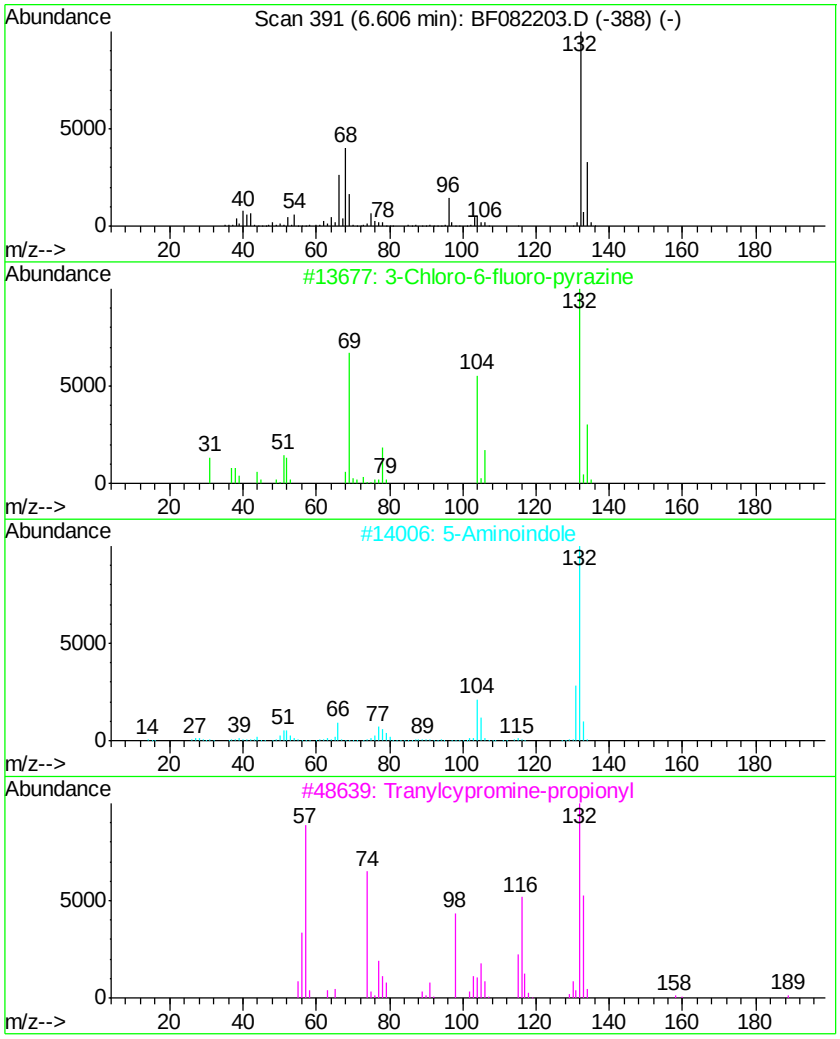
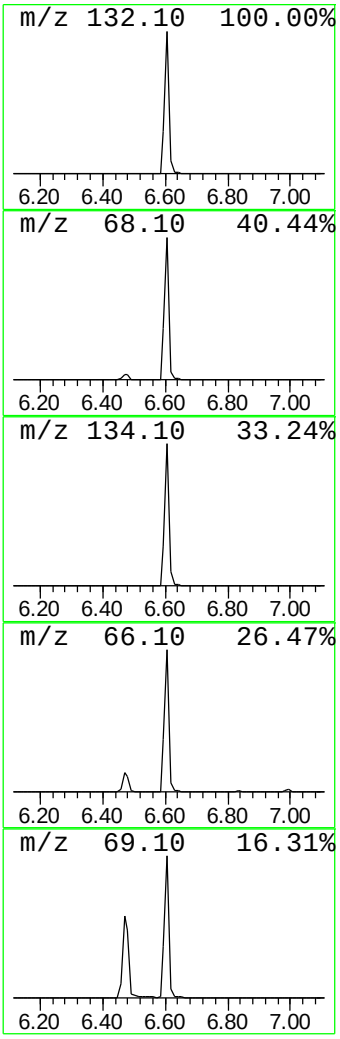
Peak Number 2 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	72.75 ng	1996560	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

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Data File : BF082203.D
Acq On : 11 Oct 2015 4:41
Operator : UM/IZ
Sample : G3979-06
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A14COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

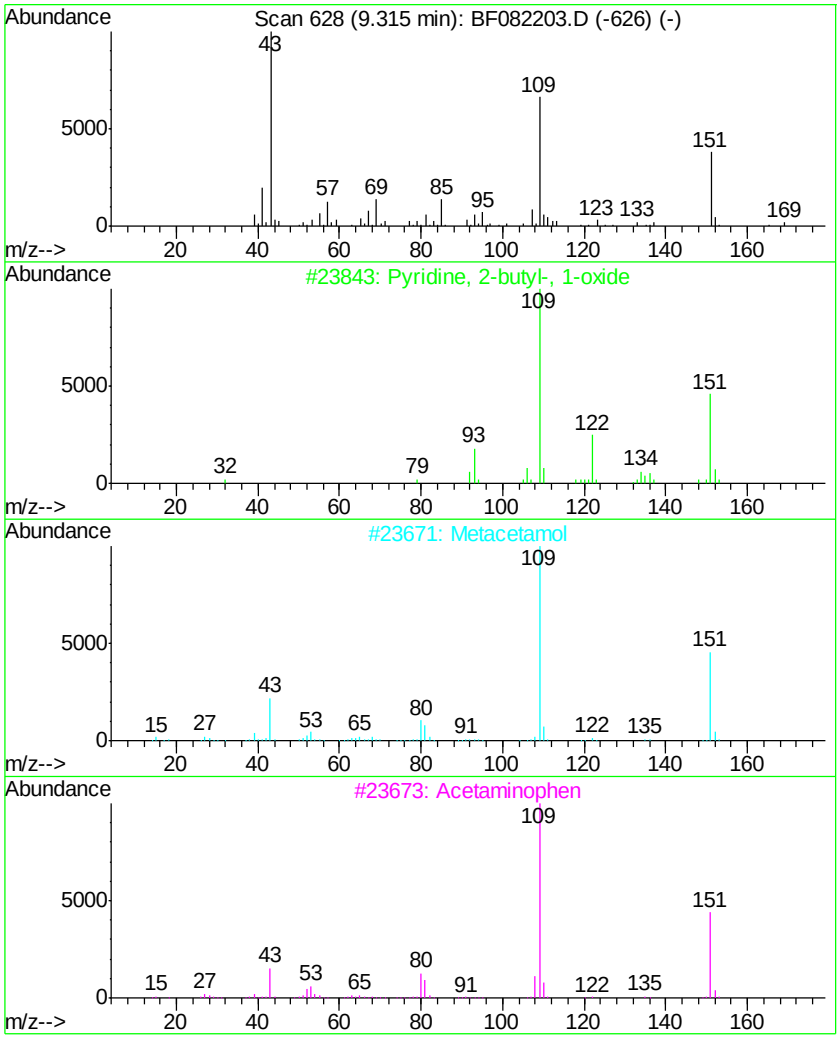
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

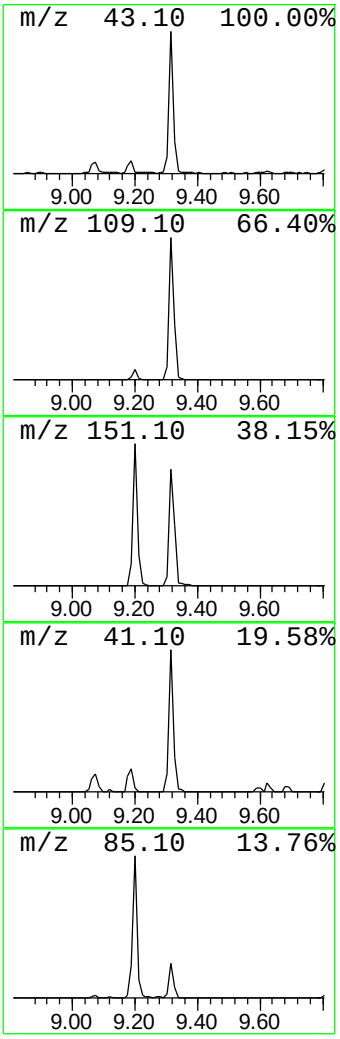
****

Peak Number 4 Pyridine, 2-butyl-, 1-oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.31	7.70 ng	320974	Acenaphthene-d10	9.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59
2	Metacetamol	151	C8H9NO2	000621-42-1	53
3	Acetaminophen	151	C8H9NO2	000103-90-2	53
4	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3	1000107-08-7	42
5	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	42





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Data File : BF082203.D
Acq On : 11 Oct 2015 4:41
Operator : UM/IZ
Sample : G3979-06
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A14COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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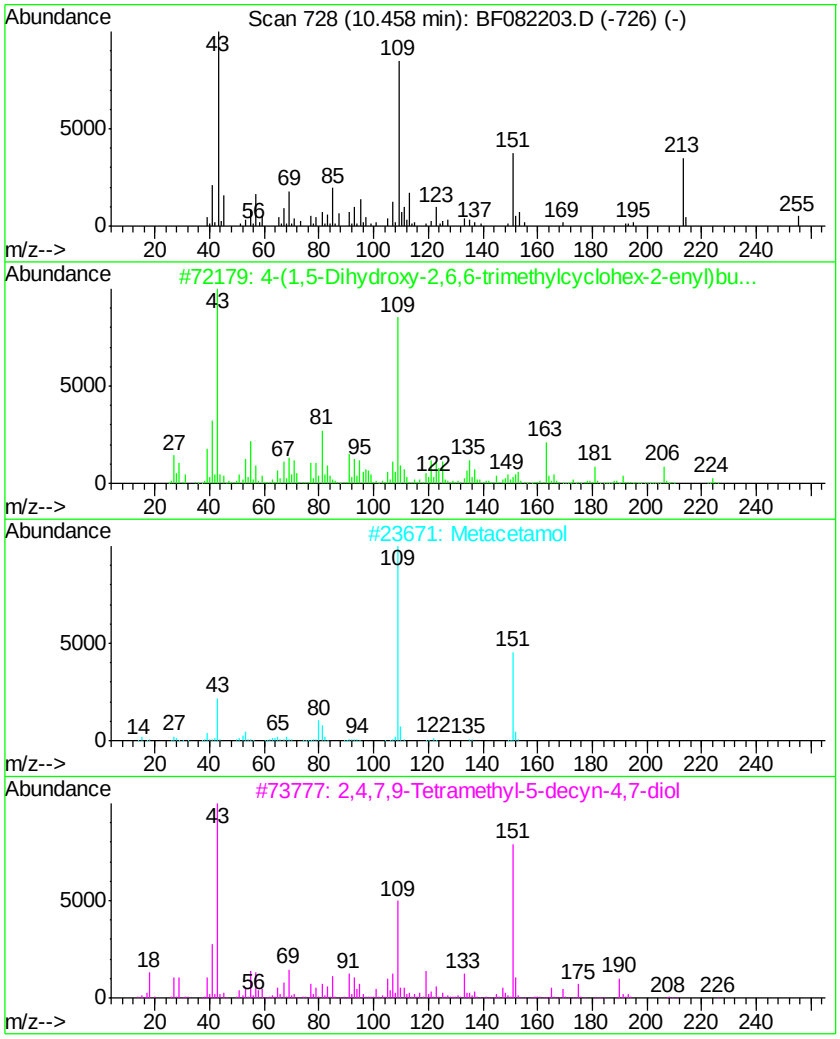
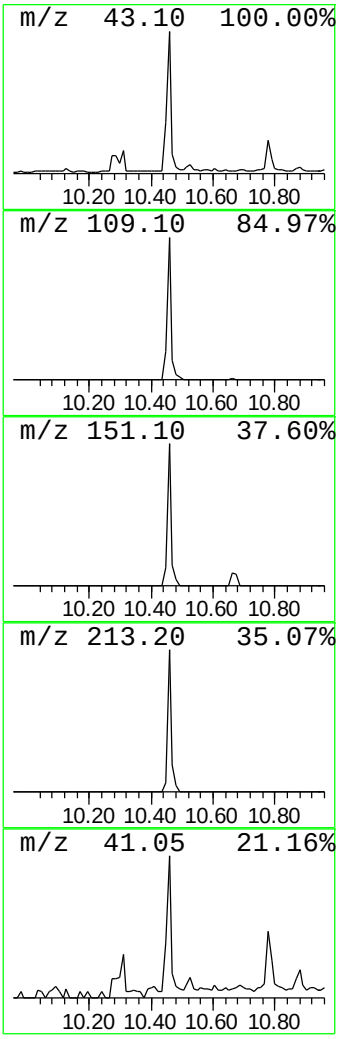
Peak Number 5 unknown10.46 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.46	4.30 ng	179330	Acenaphthene-d10	9.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(1,5-Dihydroxy-2,6,6-trimethyl...	224	C13H20O3	1000191-85-2	43
2	Metacetamol	151	C8H9NO2	000621-42-1	43
3	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	42
4	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3	1000107-08-7	38
5	1-(2-Pyrazinyl)-1-ethanol	124	C6H8N2O	094777-52-3	38





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Instrument : BNA_F
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TIC Library : C:\DATABASE\NIST02.L
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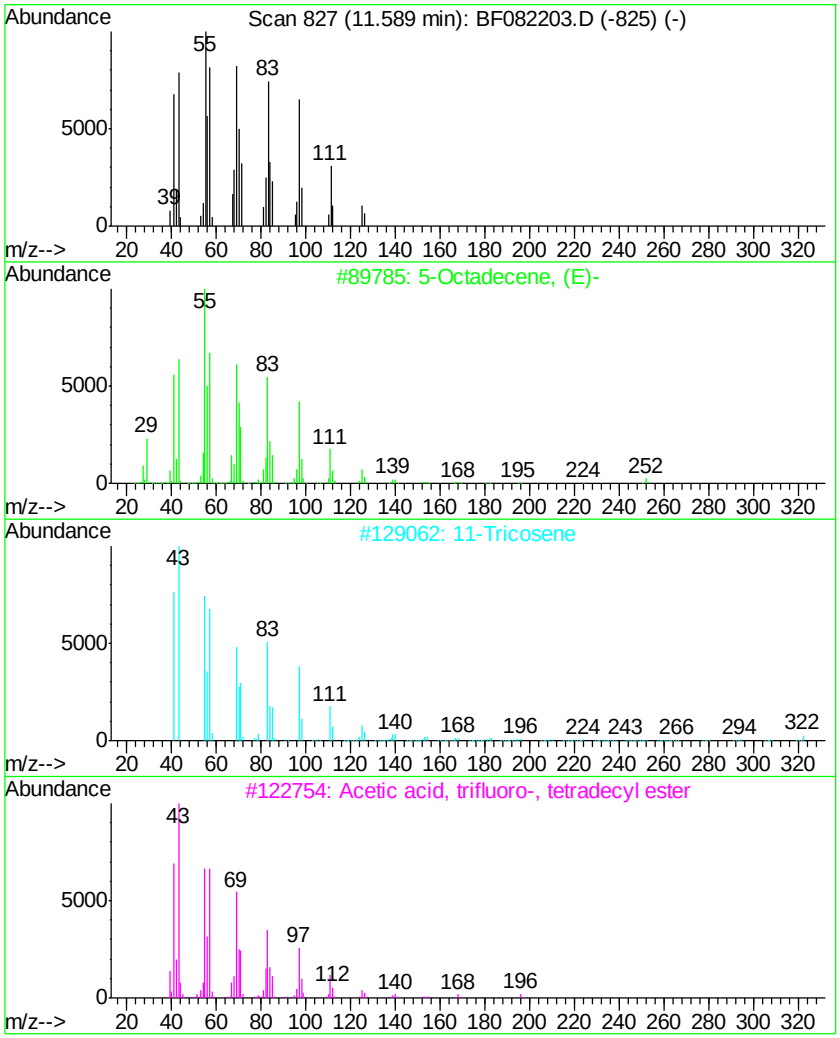
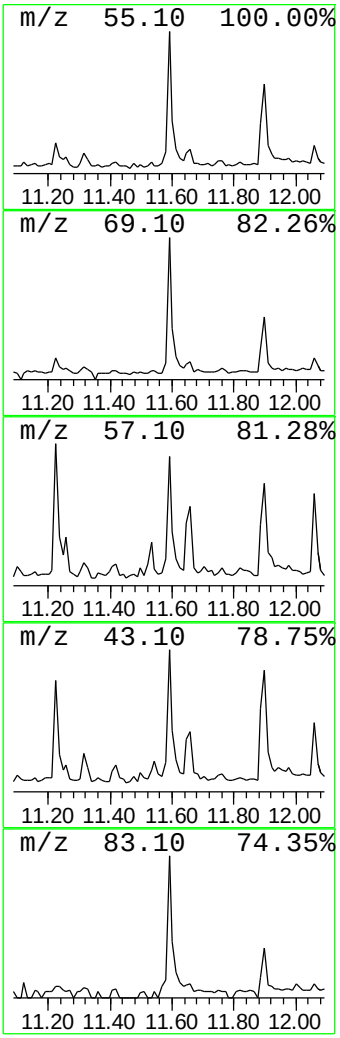
Peak Number 6 5-Octadecene, (E)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.59	2.49 ng	100898	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	91
2	11-Tricosene	322	C23H46	052078-56-5	91
3	Acetic acid, trifluoro-, tetrade...	310	C16H29F3O2	006222-02-2	90
4	9-Octadecene, (E)-	252	C18H36	007206-25-9	87
5	Pentafluoropropionic acid, dodec...	332	C15H25F5O2	006222-04-4	87





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Instrument : BNA_F
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TIC Library : C:\DATABASE\NIST02.L
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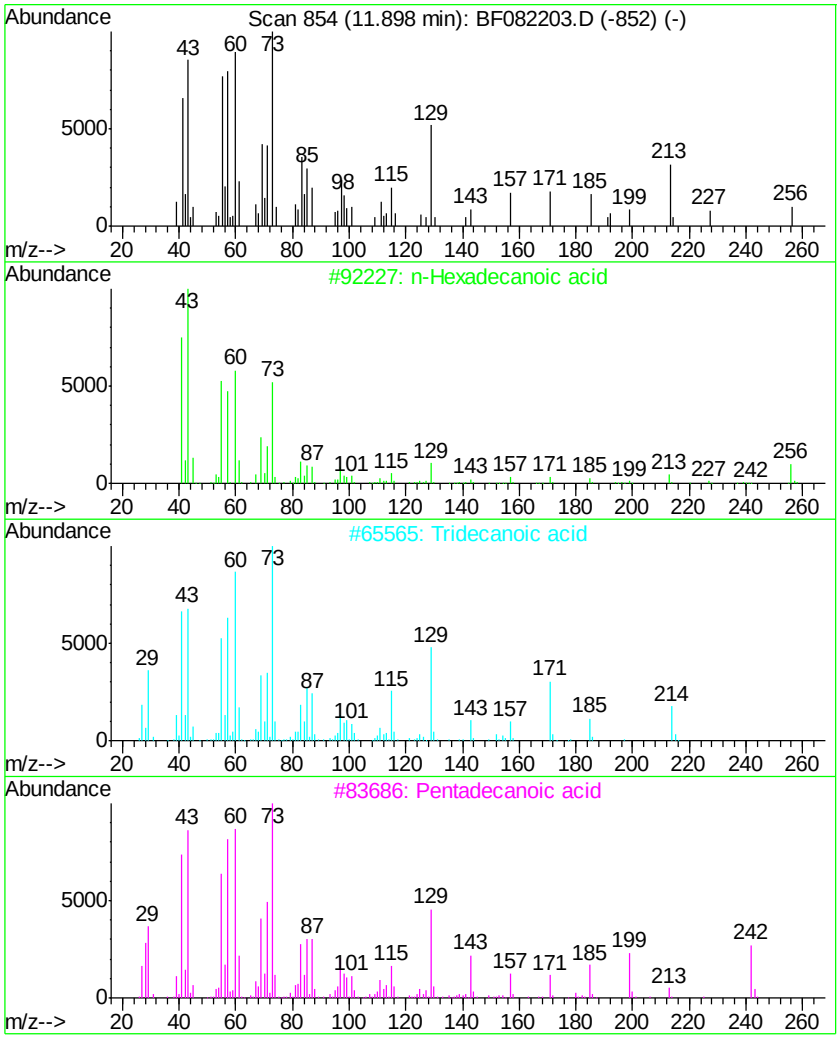
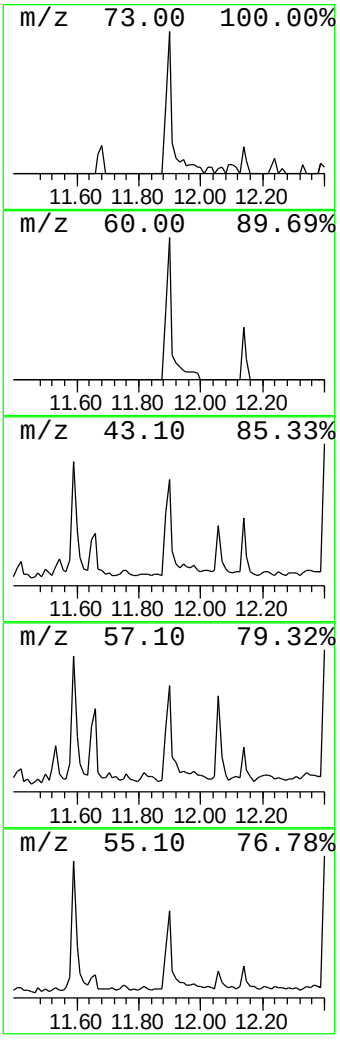
Peak Number 7 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	2.72 ng	109972	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Tridecanoic acid	214	C13H26O2	000638-53-9	76
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
5	Dodecanoic acid	200	C12H24O2	000143-07-7	47





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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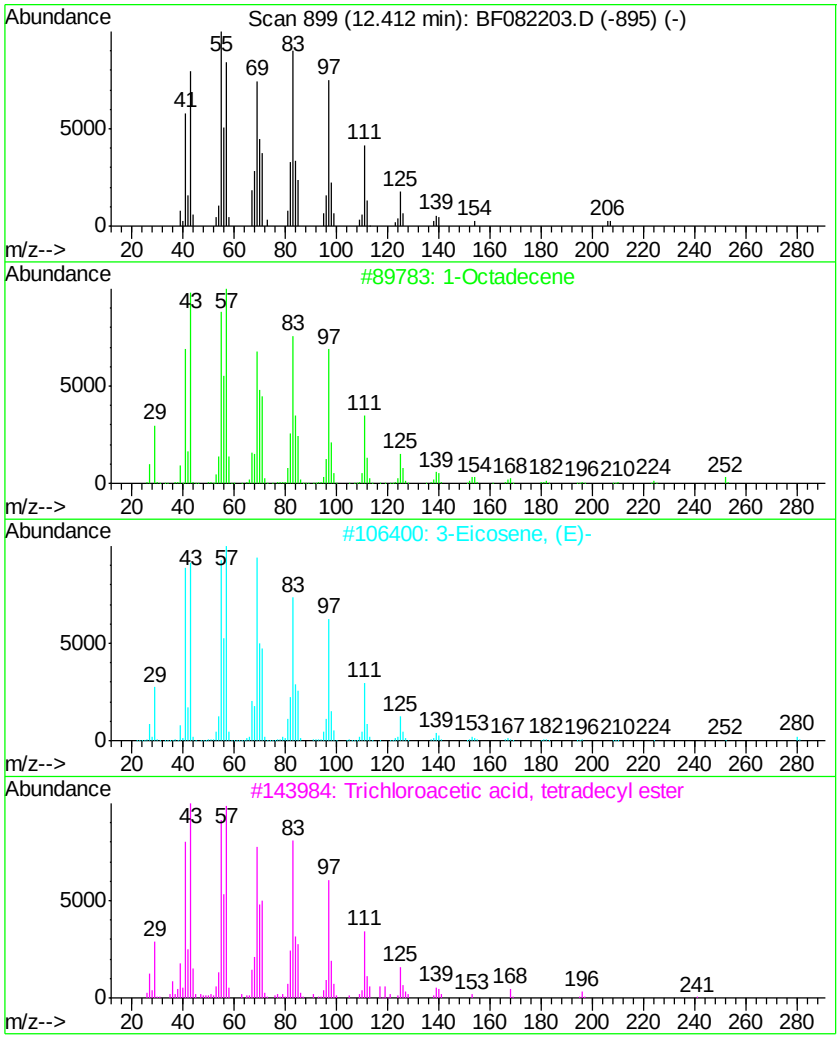
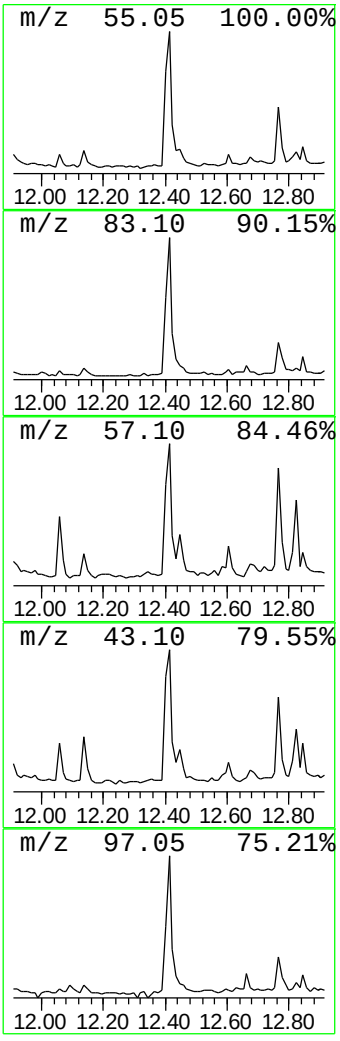
Peak Number 8 1-Octadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.41	6.28 ng	254213	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	93
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
4	1-Hexadecanol	242	C16H34O	036653-82-4	91
5	5-Octadecene, (E)-	252	C18H36	007206-21-5	91





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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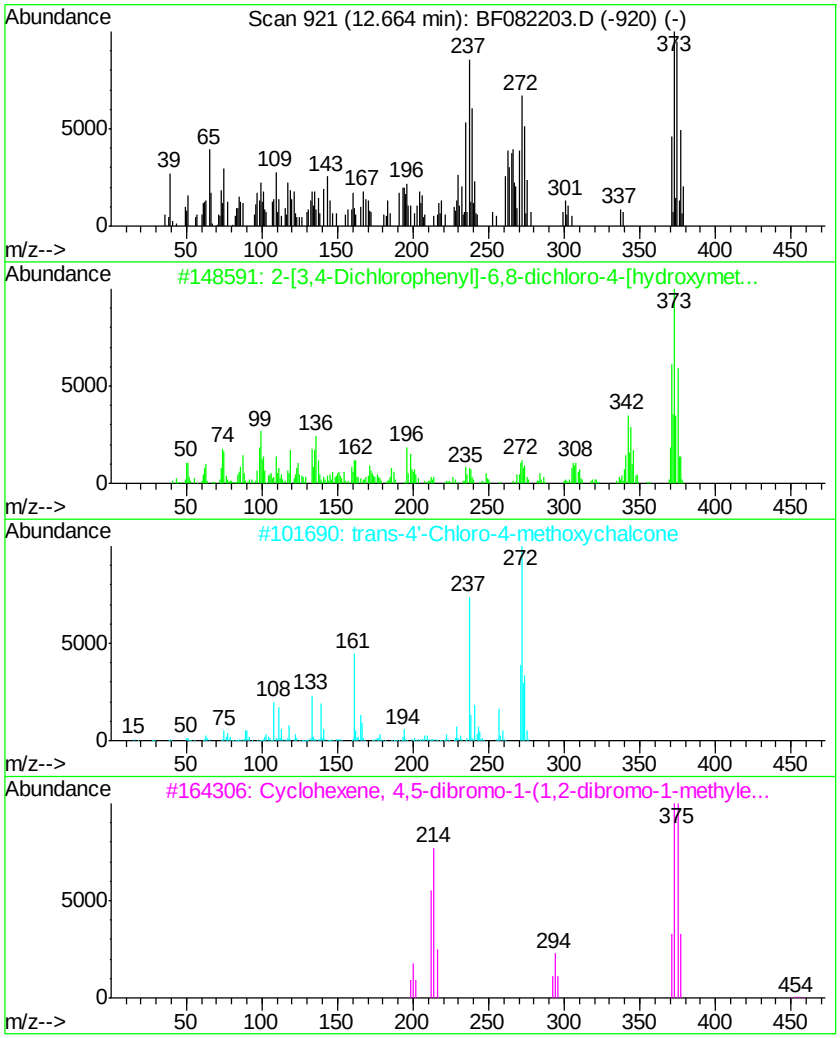
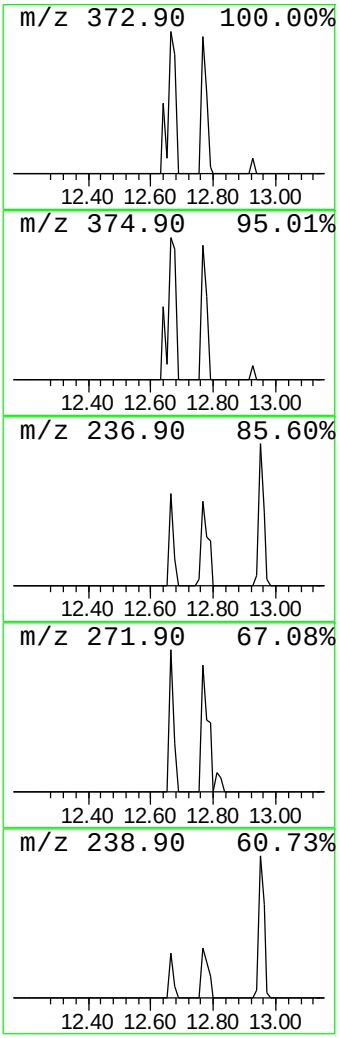
Peak Number 9 unknown12.66 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.66	3.59 ng	145336	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[3,4-Dichlorophenyl]-6,8-dichl...	371	C16H9Cl4NO	038599-01-8	22
2	trans-4'-Chloro-4-methoxychalcone	272	C16H13ClO2	006552-63-2	15
3	Cyclohexene, 4,5-dibromo-1-(1,2-...	450	C10H14Br4	070168-60-4	12
4	4-Chloro-2-[3,4-dichlorophenyl]-...	272	C11H7Cl3N2	1000253-43-6	11
5	N-(2-Fluoro-phenyl)-2-oxo-2-[N'-...	375	C18H18FN3O5	1000295-53-2	10





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101015\
Data File : BF082203.D
Acq On : 11 Oct 2015 4:41
Operator : UM/IZ
Sample : G3979-06
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A14COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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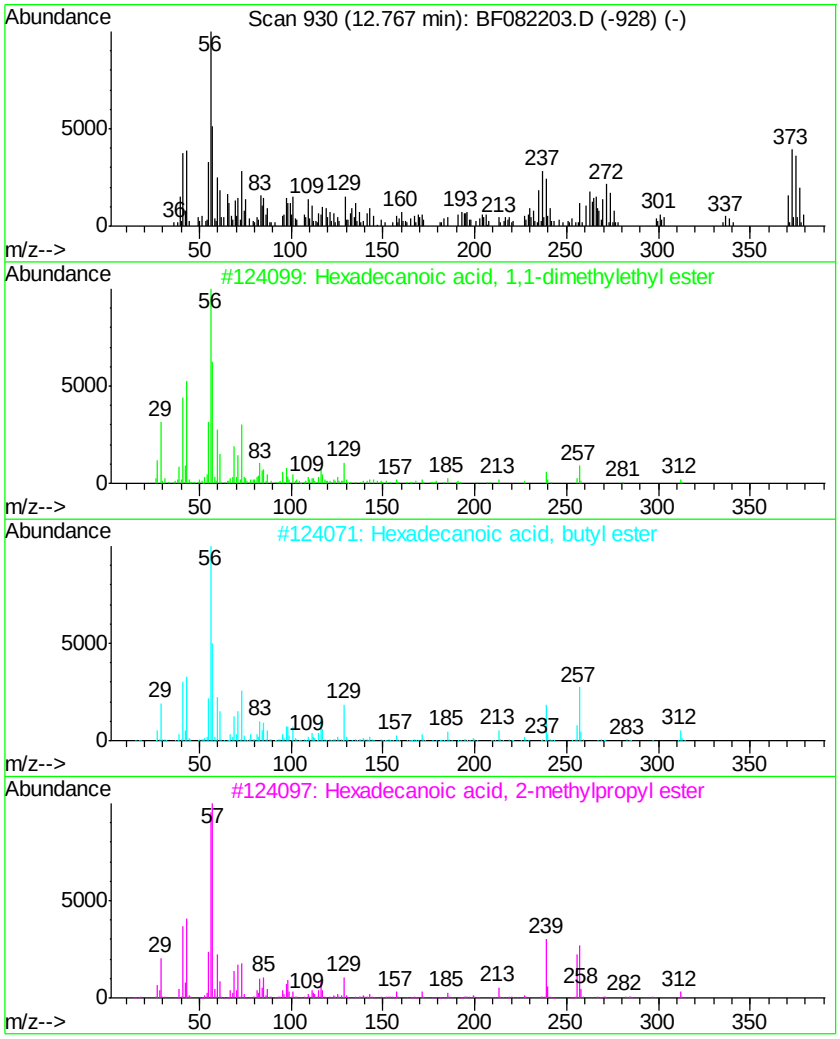
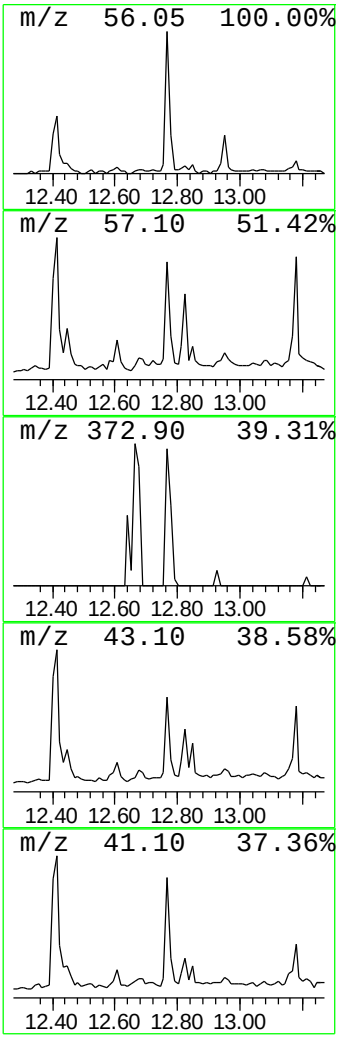
Peak Number 10 unknown12.77 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	9.95 ng	332538	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	30
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	25
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	22
4	3,4,4,6-Tetramethyl-2-(m-chlorop...	266	C14H19ClN2O	053004-31-2	12
5	3-(antipyrin-4-yl)-5-(5-nitrosal...	468	C21H16N4O5S2	314275-32-6	12





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Instrument : BNA_F
ClientSampleId : A14COMP

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

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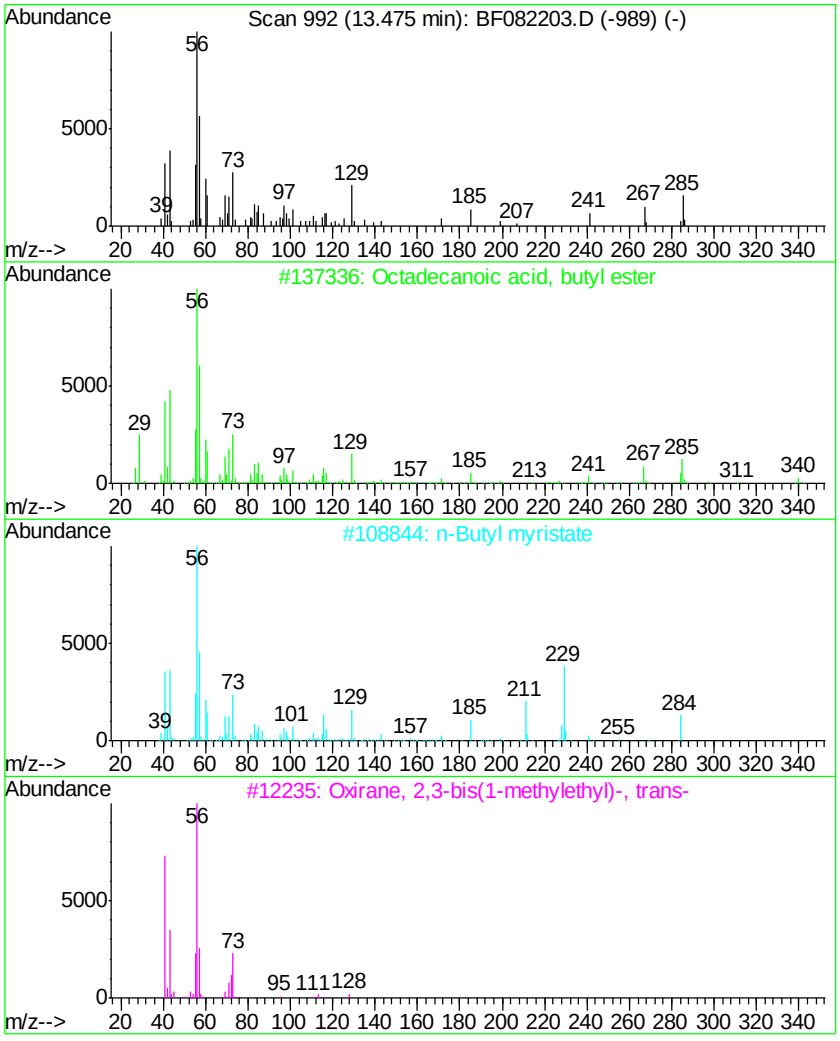
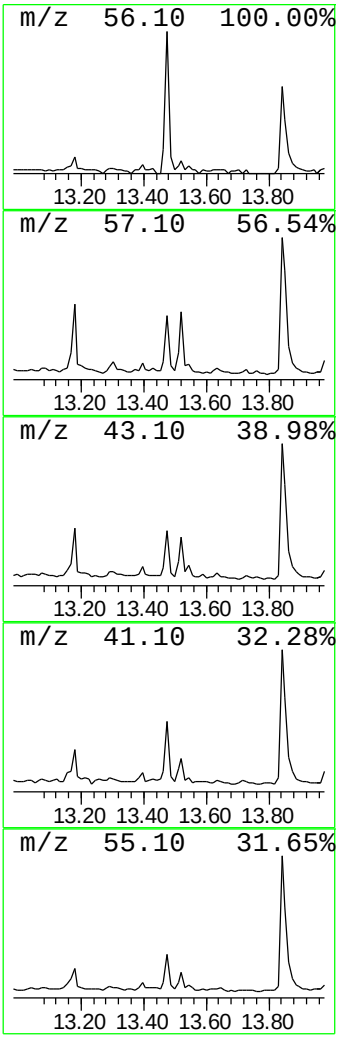
Peak Number 11 Octadecanoic acid, butyl ester Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	2.37 ng	79280	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2	n-Butyl myristate	284	C18H36O2	000110-36-1	72
3	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	38
4	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35
5	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32





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Data File : BF082203.D
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Operator : UM/IZ
Sample : G3979-06
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A14COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
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TIC Integration Parameters: LSCINT.P

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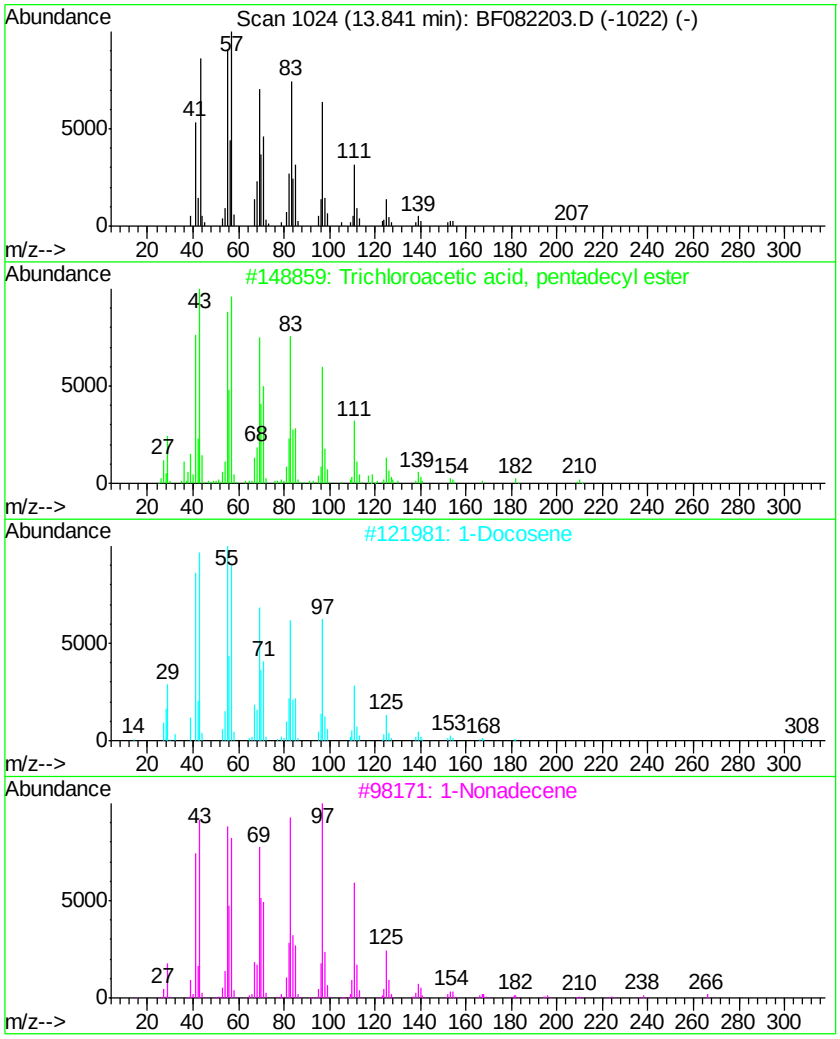
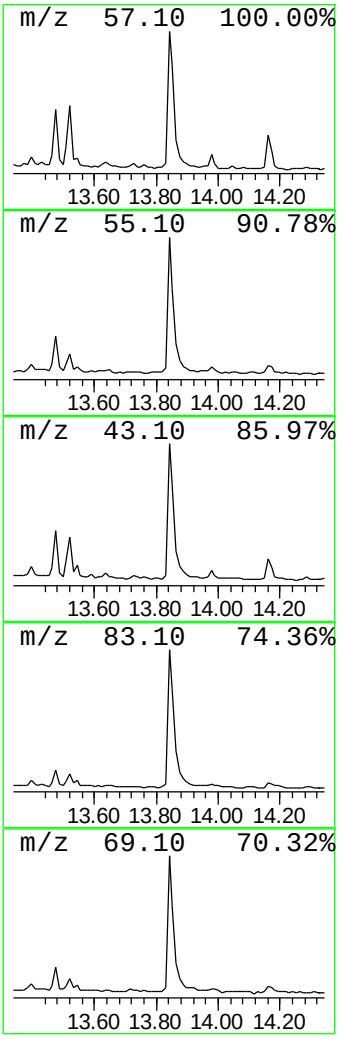
Peak Number 12 Trichloroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	8.79 ng	293681	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
2	1-Docosene	308	C22H44	001599-67-3	94
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101015\
Data File : BF082203.D
Acq On : 11 Oct 2015 4:41
Operator : UM/IZ
Sample : G3979-06
Misc :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.02	42.5	ng	1164960	1	6.83	548872	20.0
unknown6.61	6.61	72.8	ng	1996560	1	6.83	548872	20.0
Pyridine, 2-butyl...	9.31	7.7	ng	320974	3	9.87	834210	20.0
unknown10.46	10.46	4.3	ng	179330	3	9.87	834210	20.0
5-Octadecene, (E)-	11.59	2.5	ng	100898	4	11.36	809939	20.0
n-Hexadecanoic acid	11.90	2.7	ng	109972	4	11.36	809939	20.0
1-Octadecene	12.41	6.3	ng	254213	4	11.36	809939	20.0
unknown12.66	12.66	3.6	ng	145336	4	11.36	809939	20.0
unknown12.77	12.77	9.9	ng	332538	5	14.00	668276	20.0
Octadecanoic acid...	13.48	2.4	ng	79280	5	14.00	668276	20.0
Trichloroacetic a...	13.84	8.8	ng	293681	5	14.00	668276	20.0