

Data Path : Z:\HPCHEM1\BNA G\DATA\BG091815\
 Data File : BG018754.D
 Acq On : 18 Sep 2015 1:31
 Operator : TP
 Sample : G3679-07
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 WCSB3W

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_G\METHODS\8270-BG091115.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.103	40	45	52	rBV	63793	110747	3.06%	0.578%
2	3.180	53	58	76	rVB	1307643	1808768	50.05%	9.439%
3	5.101	379	385	393	rBV	113487	171192	4.74%	0.893%
4	5.571	458	465	477	rBV	372261	604007	16.71%	3.152%
5	7.163	729	736	749	rVB	264032	444774	12.31%	2.321%
6	7.533	791	799	808	rBV	701930	1145963	31.71%	5.980%
7	7.998	871	878	886	rVB	139610	235446	6.51%	1.229%
8	8.327	926	934	941	rBV	581331	1010209	27.95%	5.272%
9	9.161	1068	1076	1084	rVB	492601	845445	23.39%	4.412%
10	10.806	1348	1356	1363	rBV	216472	384139	10.63%	2.005%
11	13.250	1763	1772	1781	rBV	1626284	2475324	68.49%	12.917%
12	14.073	1906	1912	1917	rBV	49457	70011	1.94%	0.365%
13	14.625	1997	2006	2014	rBV2	390531	641125	17.74%	3.346%
14	15.036	2071	2076	2085	rBV2	85888	141154	3.91%	0.737%
15	15.436	2136	2144	2147	rBV3	46433	76554	2.12%	0.399%
16	16.112	2252	2259	2274	rBV	1315569	2012495	55.68%	10.502%
17	16.294	2284	2290	2299	rBV	93179	165608	4.58%	0.864%
18	17.110	2424	2429	2434	rBV3	20764	38343	1.06%	0.200%
19	17.369	2467	2473	2481	rBV	563351	832685	23.04%	4.345%
20	18.256	2619	2624	2633	rBV2	118179	187381	5.18%	0.978%
21	19.525	2836	2840	2848	rBV2	87728	140814	3.90%	0.735%
22	19.978	2911	2917	2923	rBV	2873644	3614257	100.00%	18.861%
23	21.276	3135	3138	3151	rVB8	49690	98123	2.71%	0.512%
24	21.629	3192	3198	3207	rVB	596580	959516	26.55%	5.007%
25	24.819	3731	3741	3753	rVB2	327064	949019	26.26%	4.952%

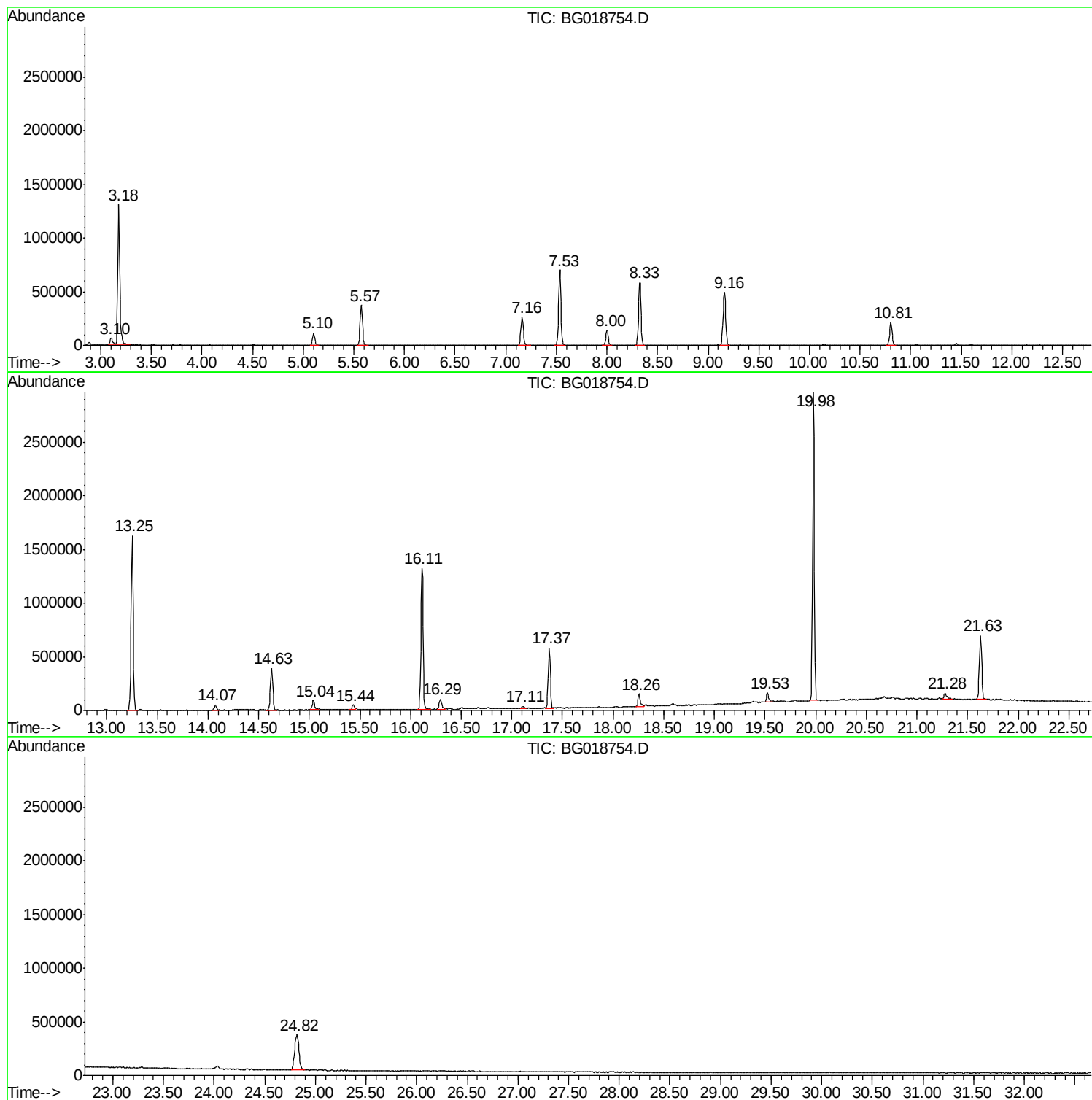
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG091115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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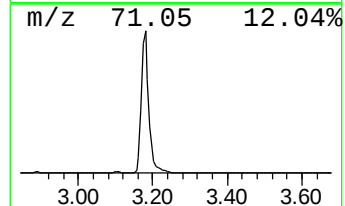
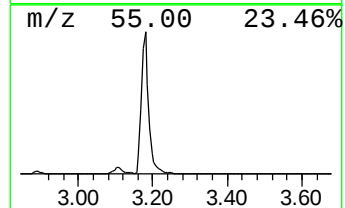
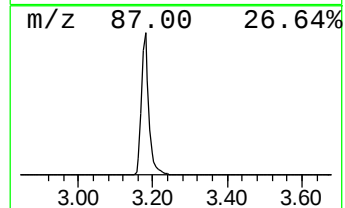
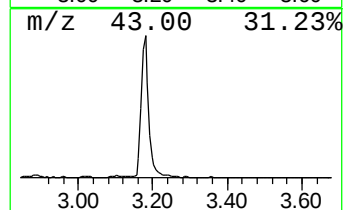
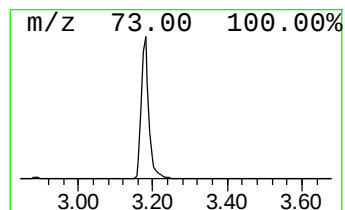
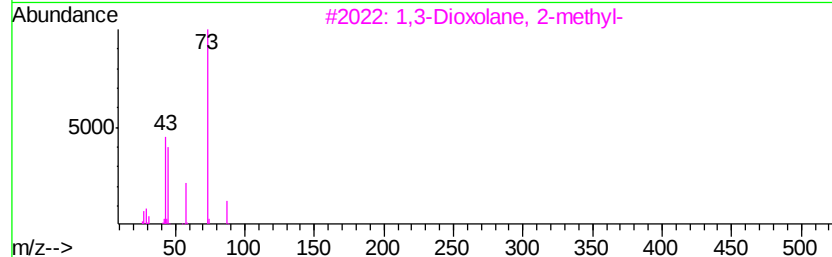
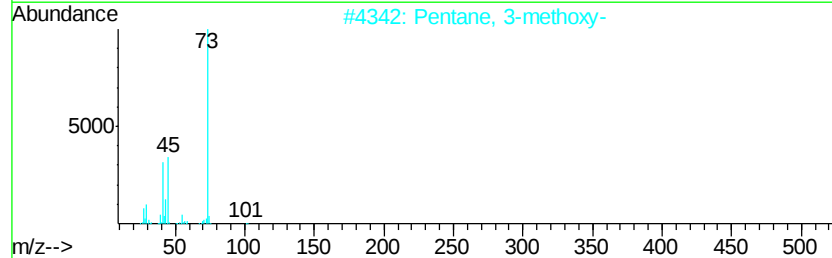
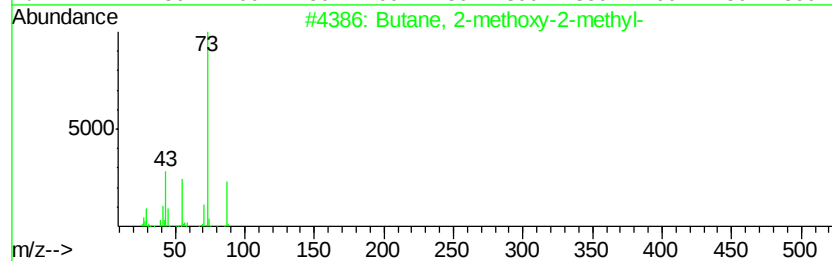
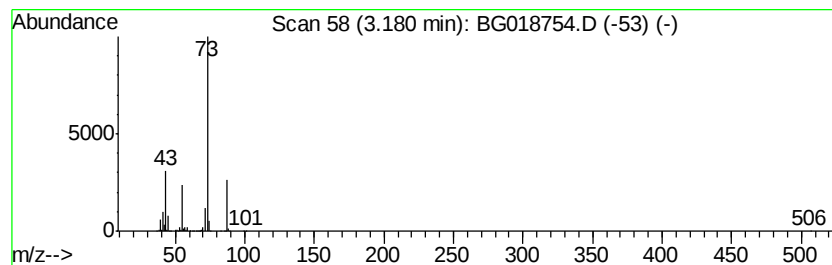
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG091115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	153.65 ng	1808770	1,4-Dichlorobenzene-d4	8.00

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	90
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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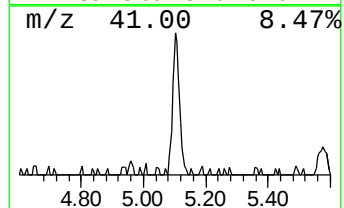
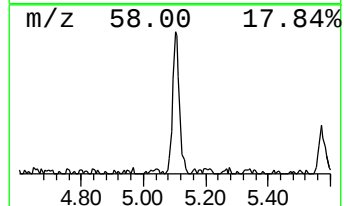
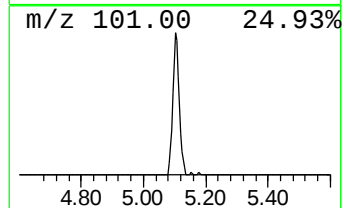
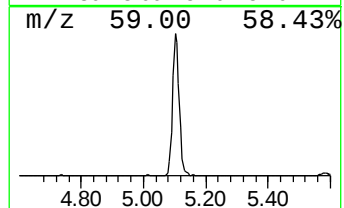
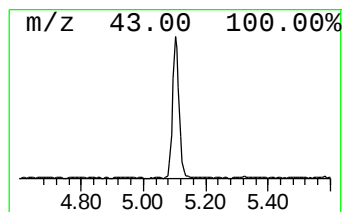
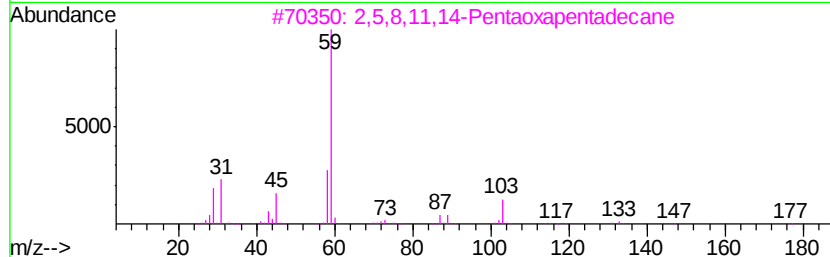
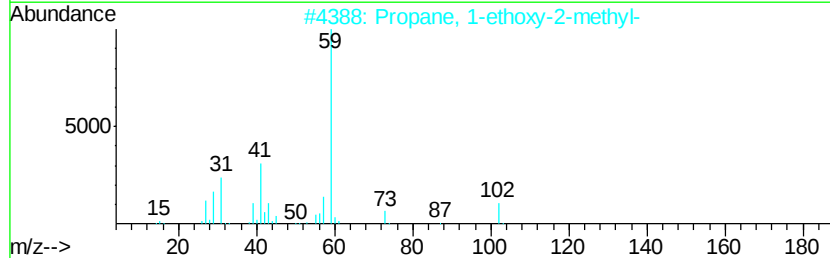
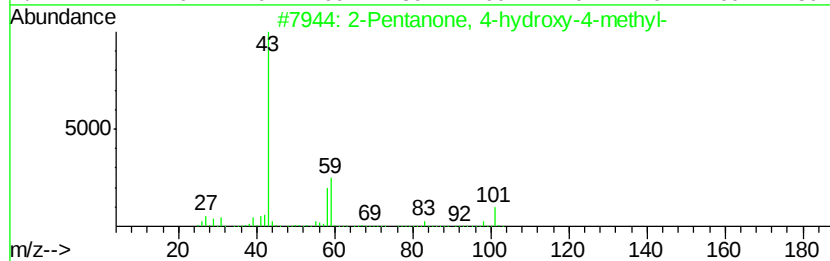
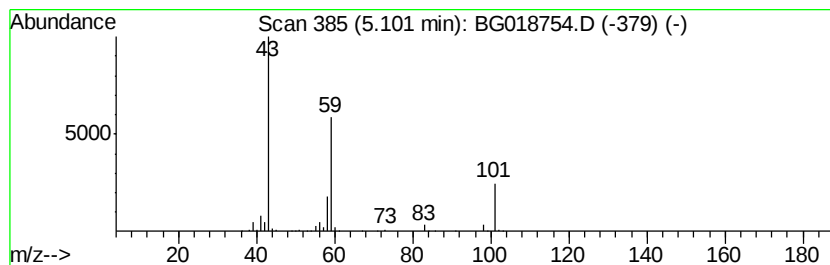
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 unknown5.10 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	14.54 ng	171192	1,4-Dichlorobenzene-d4	8.00

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25
3			2,5,8,11,14-Pentaoxapentadecane	222	C10H22O5	000143-24-8	25
4			1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	23
5			2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	23



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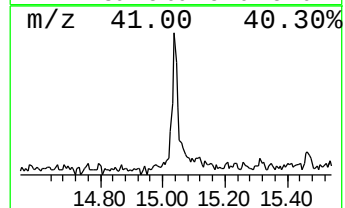
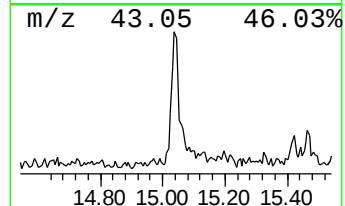
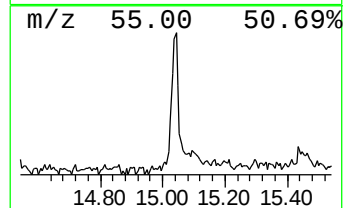
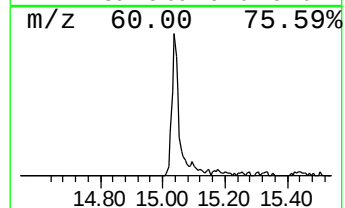
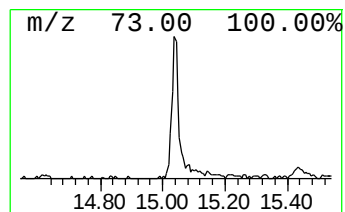
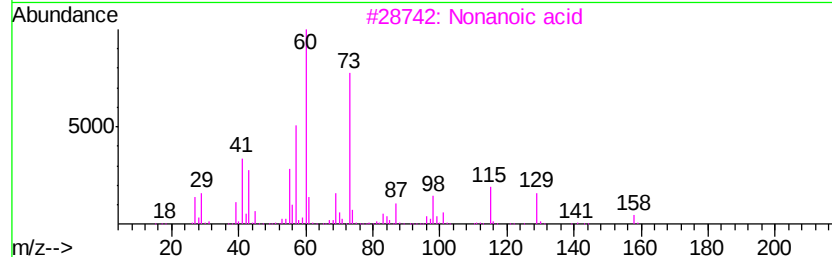
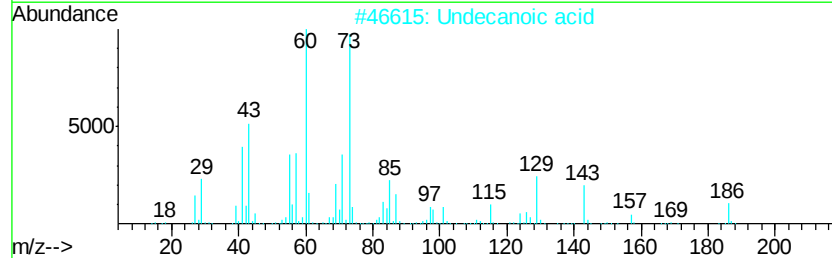
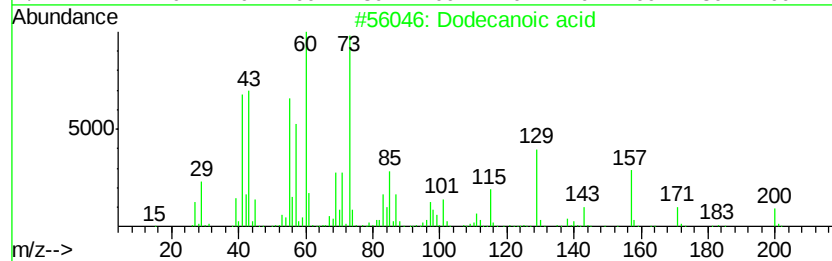
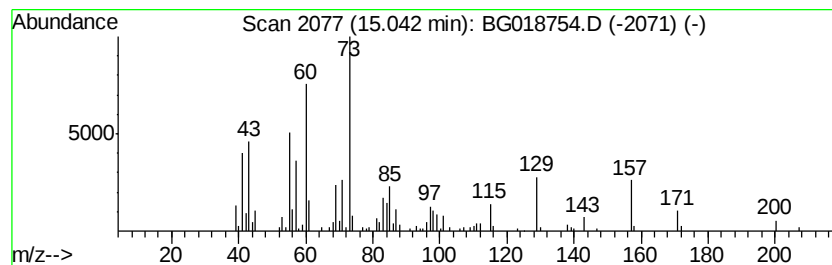
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Peak Number 6 Dodecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.04	4.40 ng	141154	Acenaphthene-d10		14.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	91
2			Undecanoic acid	186	C11H22O2	000112-37-8	59
3			Nonanoic acid	158	C9H18O2	000112-05-0	50
4			D-Glucose, 4-O-.alpha.-D-glucopy...	342	C12H22O11	000069-79-4	47
5			d-Glucohexodialdose	178	C6H10O6	1000149-19-1	43



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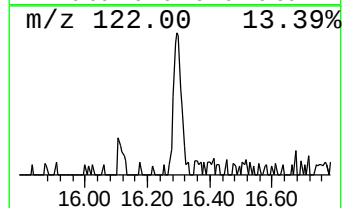
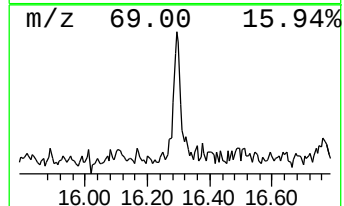
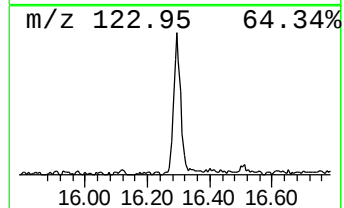
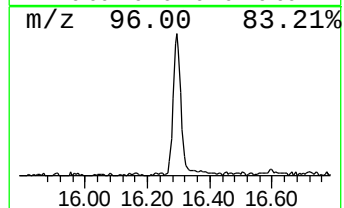
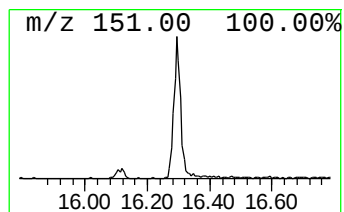
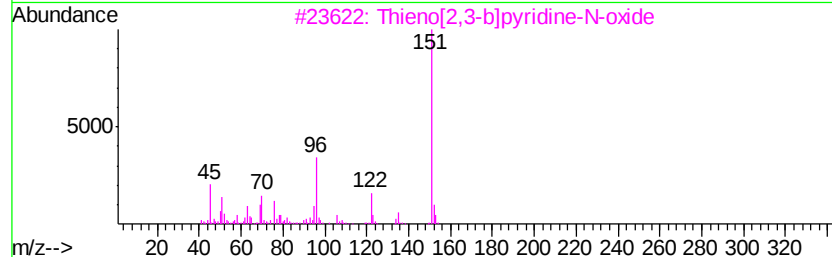
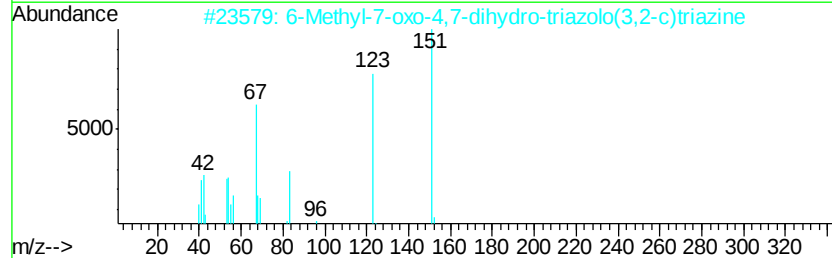
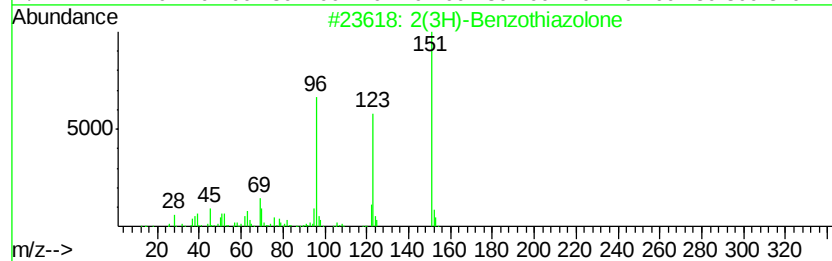
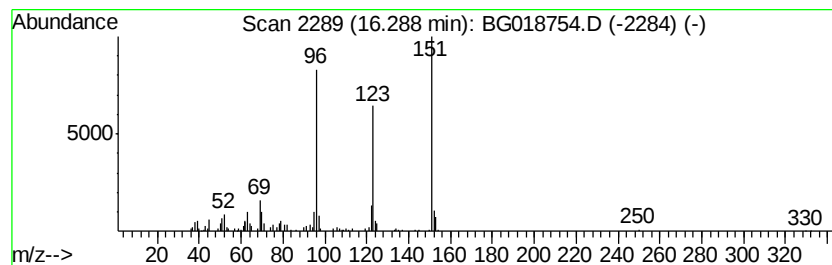
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Peak Number 7 2(3H)-Benzothiazolone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.29	3.98 ng	165608	Phenanthrene-d10	17.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	94
2		6-Methyl-7-oxo-4,7-dihydro-triaz...	151	C5H5N5O	057250-39-2	50
3		Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	50
4		1,4-Benzenediol, 2-(1,1-dimethyl...	166	C10H14O2	001948-33-0	50
5		1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	43



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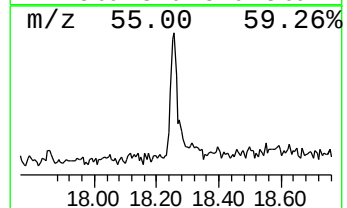
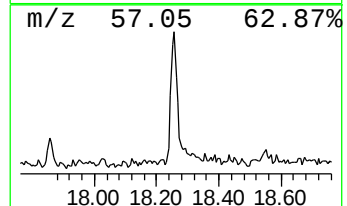
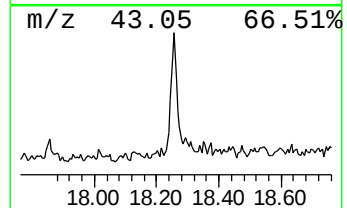
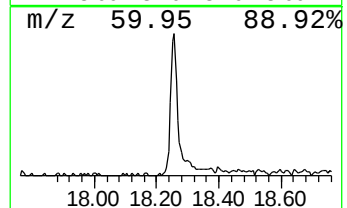
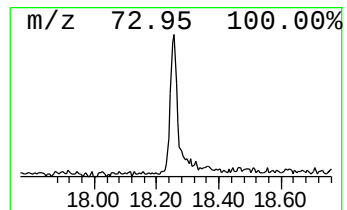
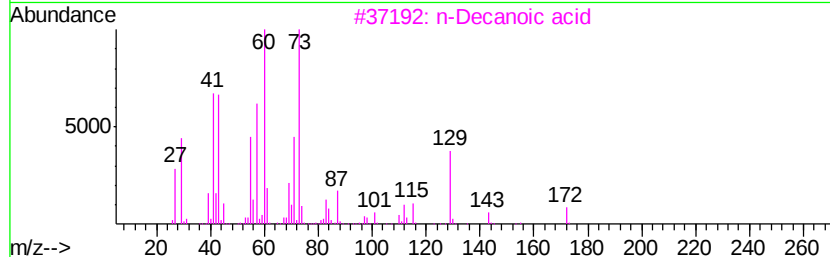
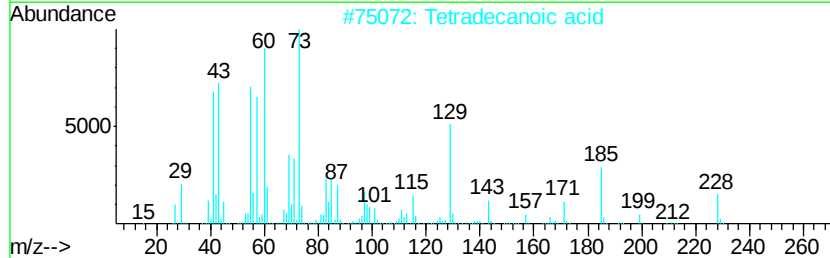
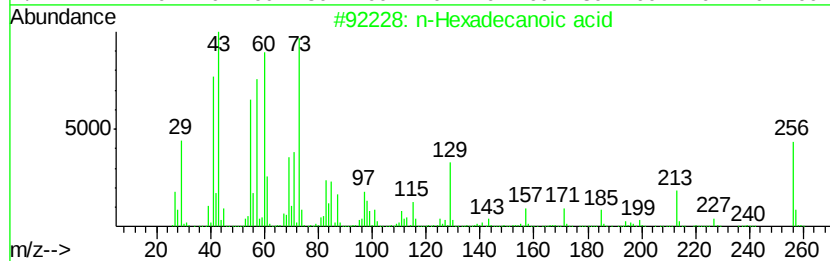
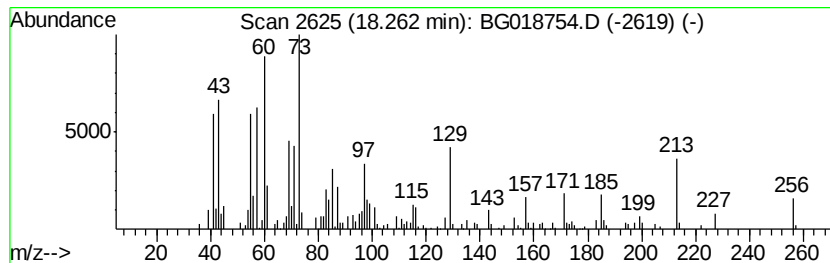
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 8 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.26	4.50 ng	187381	Phenanthrene-d10	17.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	n-Decanoic acid	172	C10H20O2	000334-48-5	64
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	Undecanoic acid	186	C11H22O2	000112-37-8	58



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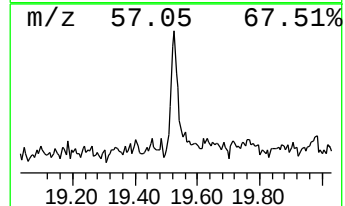
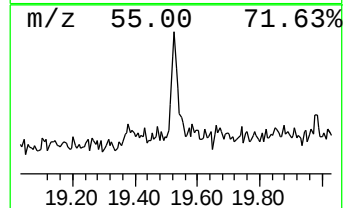
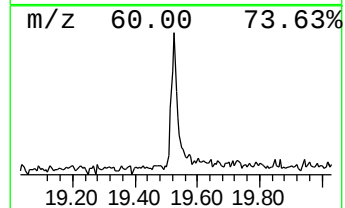
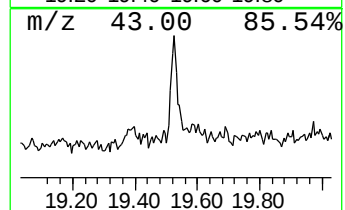
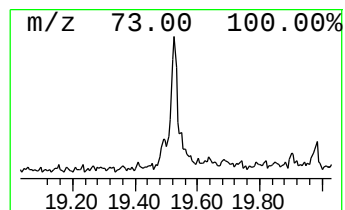
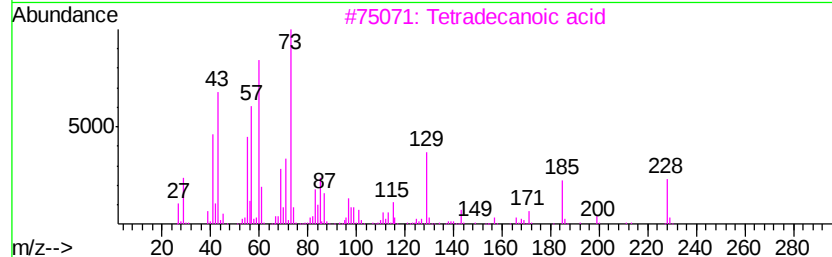
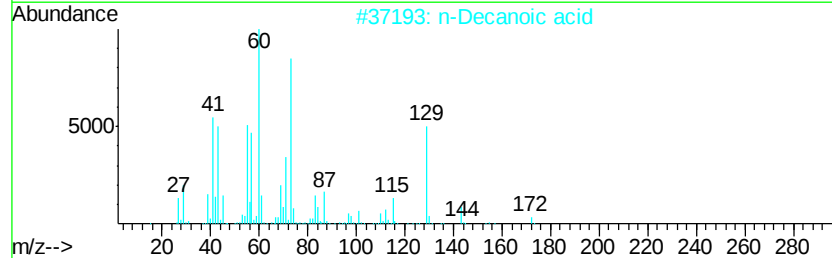
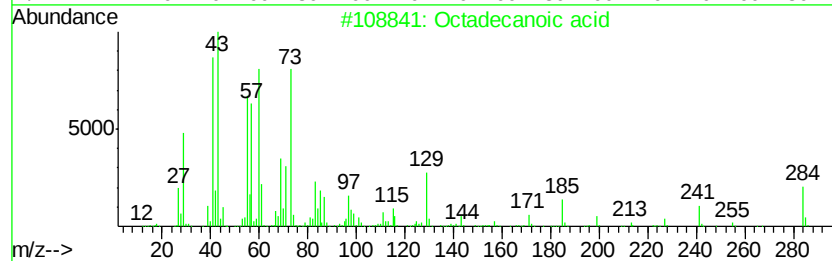
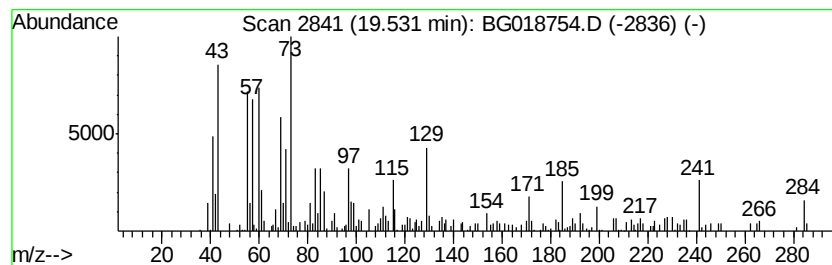
Instrument :
BNA_G
ClientSampleId :
WCSB3W

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG091115.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 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.		
19.53	2.94 ng	140814	Chrysene-d12		21.63		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	94
2			n-Decanoic acid	172	C10H20O2	000334-48-5	50
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	50
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	43
5			11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	43



Data Path : Z:\HPCHEM1\BNA G\DATA\BG091815\
Data File : BG018754.D
Acq On : 18 Sep 2015 1:31
Operator : TP
Sample : G3679-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

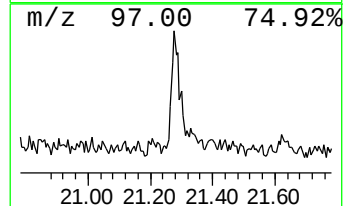
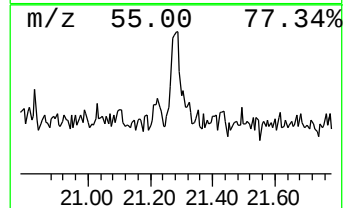
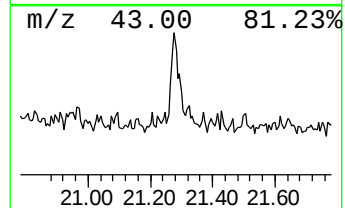
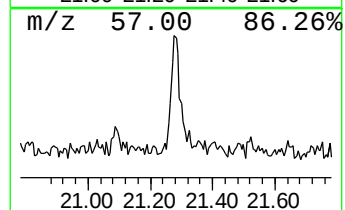
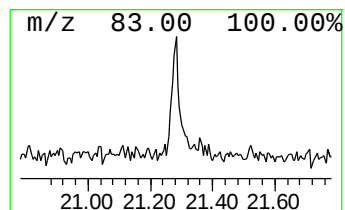
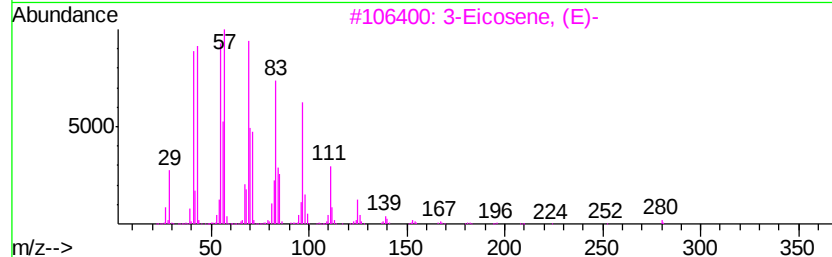
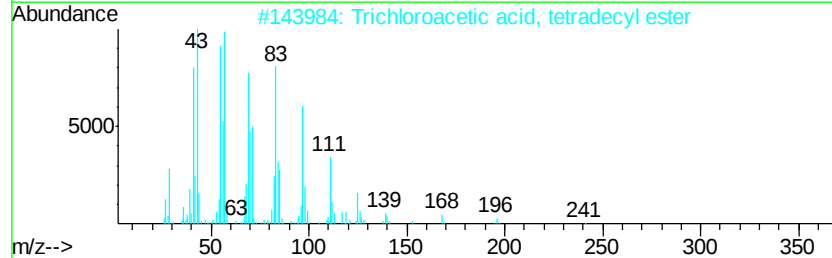
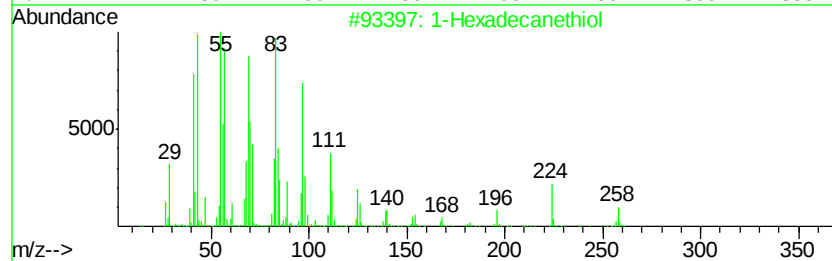
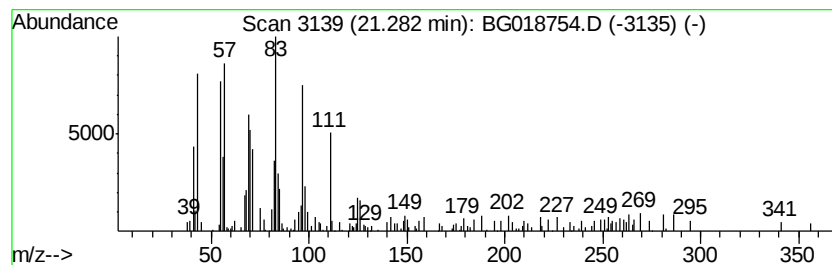
Instrument :
BNA_G
ClientSampleId :
WCSB3W

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG091115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Hexadecanethiol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.28	2.05 ng	98123	Chrysene-d12	21.63	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanethiol	258	C16H34S	002917-26-2	89
2	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	68
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	68
4	1-Heptadecanol	256	C17H36O	001454-85-9	64
5	1-Octadecanol	270	C18H38O	000112-92-5	64



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG091815\
Data File : BG018754.D
Acq On : 18 Sep 2015 1:31
Operator : TP
Sample : G3679-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WCSB3W

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.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
Butane, 2-methoxy...	3.18	153.7	ng	1808770	1	8.00	235446	20.0
unknown5.10	5.10	14.5	ng	171192	1	8.00	235446	20.0
Dodecanoic acid	15.04	4.4	ng	141154	3	14.63	641125	20.0
2(3H)-Benzothiazo...	16.29	4.0	ng	165608	4	17.37	832685	20.0
n-Hexadecanoic acid	18.26	4.5	ng	187381	4	17.37	832685	20.0
Octadecanoic acid	19.53	2.9	ng	140814	5	21.63	959516	20.0
1-Hexadecanethiol	21.28	2.0	ng	98123	5	21.63	959516	20.0