LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG060916\
Data File : BG022279.D
Acq On : 10 Jun 2016 4:31
Operator : UM/SJ
Sample : H3396-04
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : STA-942-PLATFORM(0-4)

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_G\METHODS\8270-BG060616.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	2.868	3	5	7	rVB	2143245	1510184	64.00%	10.583%
2	3.955	185	190	199	rVB	17330	31976	1.36%	0.224%
3	4.572	289	295	308	rBV	364318	637506	27.02%	4.468%
4	5.189	393	400	414	rVB	88075	170023	7.20%	1.191%
5	5.671	474	482	496	rBV	432337	812160	34.42%	5.691%
6	7.281	748	756	770	rBV	436359	846610	35.88%	5.933%
7	7.651	810	819	833	rBV	544192	1048516	44.43%	7.348%
8	8.115	887	898	909	rBV	94200	185221	7.85%	1.298%
9	8.444	944	954	967	rBV	419680	825846	35.00%	5.787%
10	9.290	1089	1098	1114	rBV	300342	635052	26.91%	4.450%
11	10.935	1370	1378	1384	rBV	156806	316656	13.42%	2.219%
12	10.982	1384	1386	1394	rVB	16901	29888	1.27%	0.209%
13	13.368	1784	1792	1805	rBV	1090948	1837957	77.89%	12.880%
14	14.748	2017	2027	2035	rBV2	249217	447294	18.95%	3.135%
15	16.235	2273	2280	2297	rBV	625319	1104189	46.79%	7.738%
16	17.492	2487	2494	2505	rBV2	282052	478511	20.28%	3.353%
17	19.754	2873	2879	2886	rVB	60216	82661	3.50%	0.579%
18	20.083	2928	2935	2944	rBV	1615726	2359801	100.00%	16.537%
19	20.794	3050	3056	3062	rBV	43677	59515	2.52%	0.417%
20	21.770	3214	3222	3233	rBV2	242521	486115	20.60%	3.407%
21	25.066	3771	3783	3803	rBV2	89908	364176	15.43%	2.552%

Sum of corrected areas: 14269857

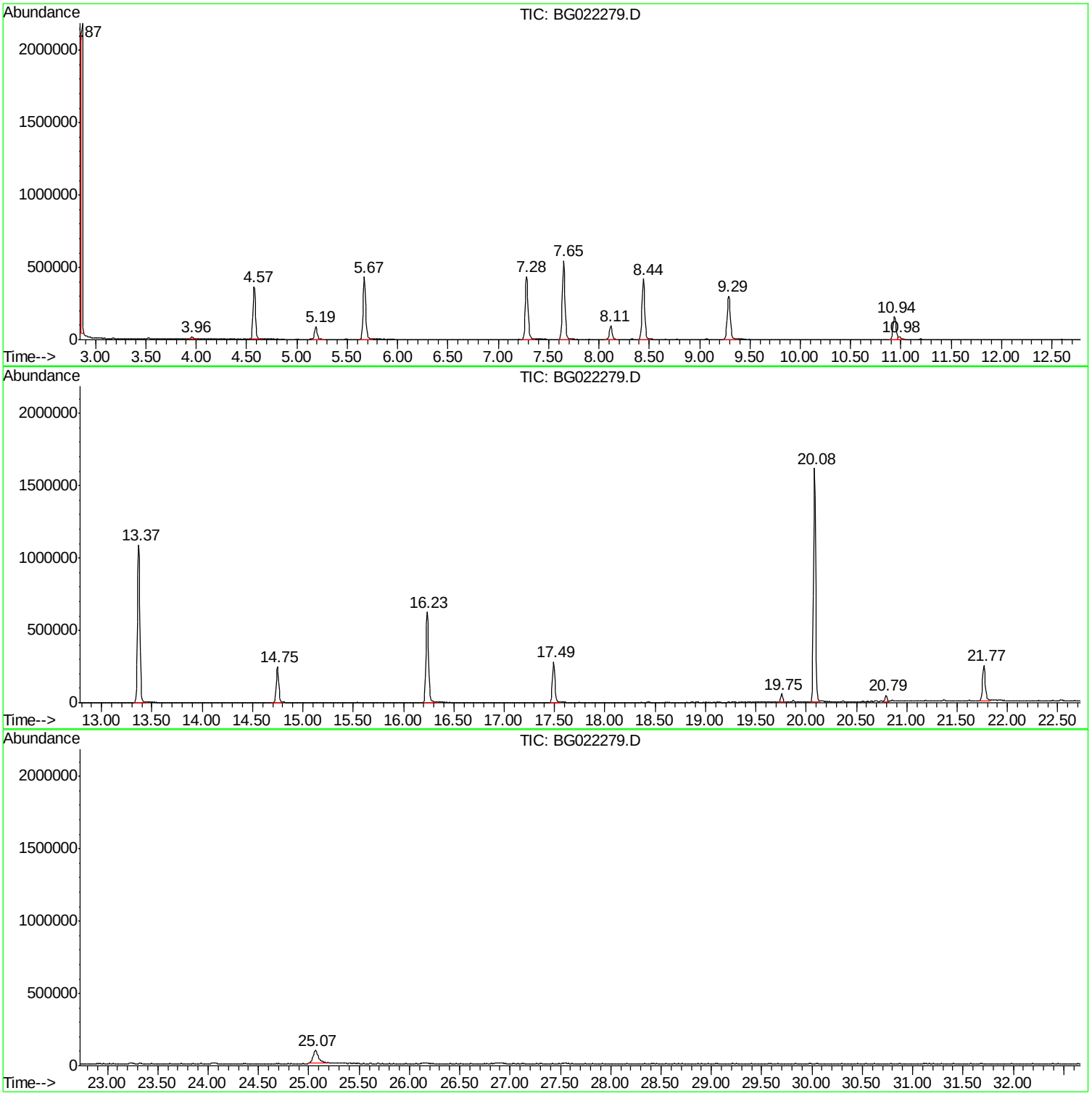
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG060916\
Data File : BG022279.D
Acq On : 10 Jun 2016 4:31
Operator : UM/SJ
Sample : H3396-04
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
STA-942-PLATFORM(0-4)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.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

Data Path : Z:\HPCHEM1\BNA G\DATA\BG060916\
Data File : BG022279.D
Acq On : 10 Jun 2016 4:31
Operator : UM/SJ
Sample : H3396-04
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
STA-942-PLATFORM(0-4)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

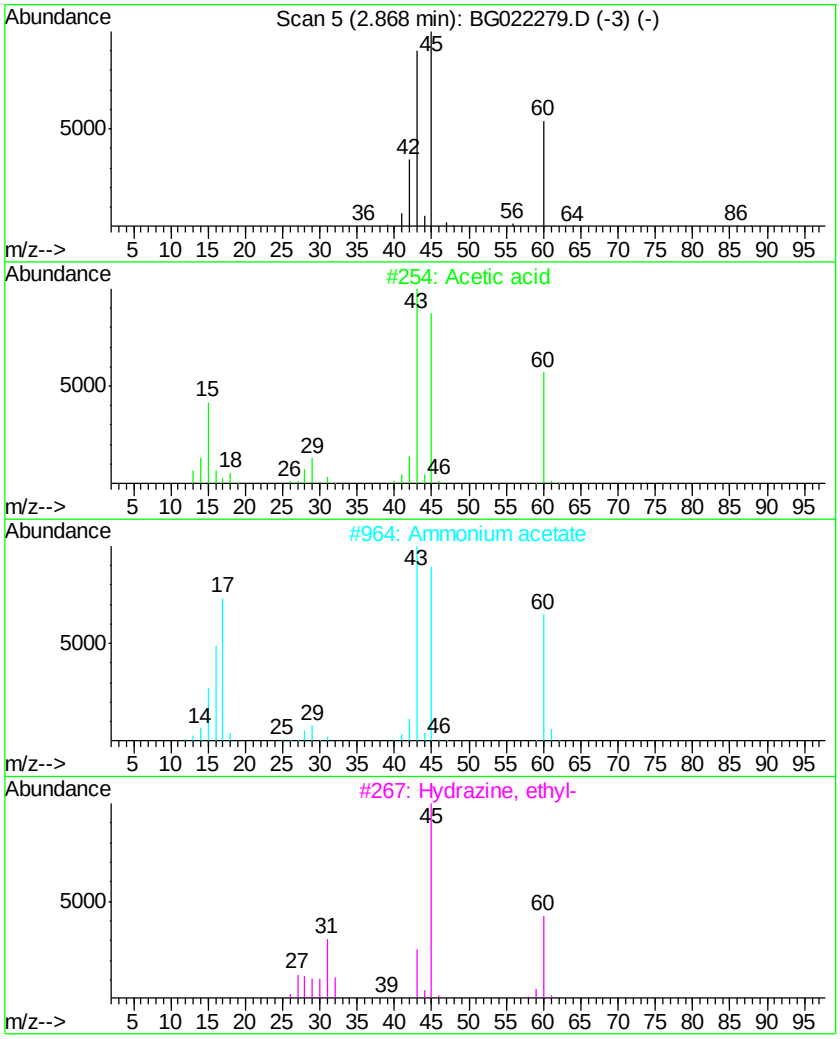
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

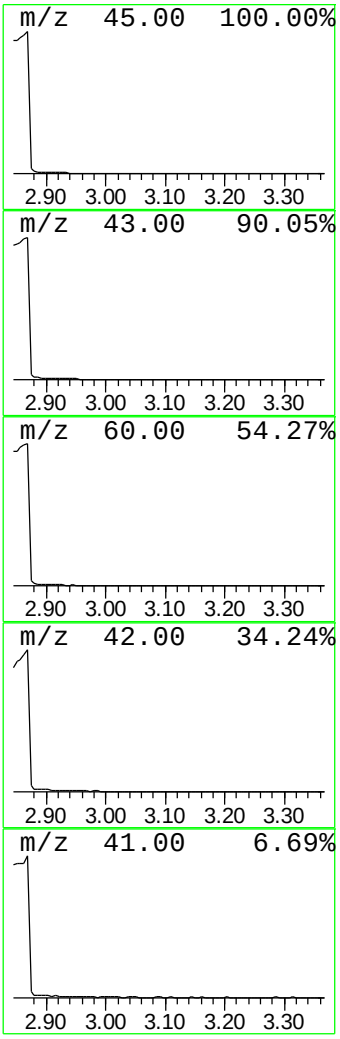
****

Peak Number 1 Acetic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.87	163.07 ng	1510180	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	86
2	Ammonium acetate	77	C2H7NO2	000631-61-8	9
3	Hydrazine, ethyl-	60	C2H8N2	000624-80-6	7
4	Thiirane	60	C2H4S	000420-12-2	7
5	Carbonyl sulfide	60	COS	000463-58-1	4





Data Path : Z:\HPCHEM1\BNA G\DATA\BG060916\
Data File : BG022279.D
Acq On : 10 Jun 2016 4:31
Operator : UM/SJ
Sample : H3396-04
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : STA-942-PLATFORM(0-4)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

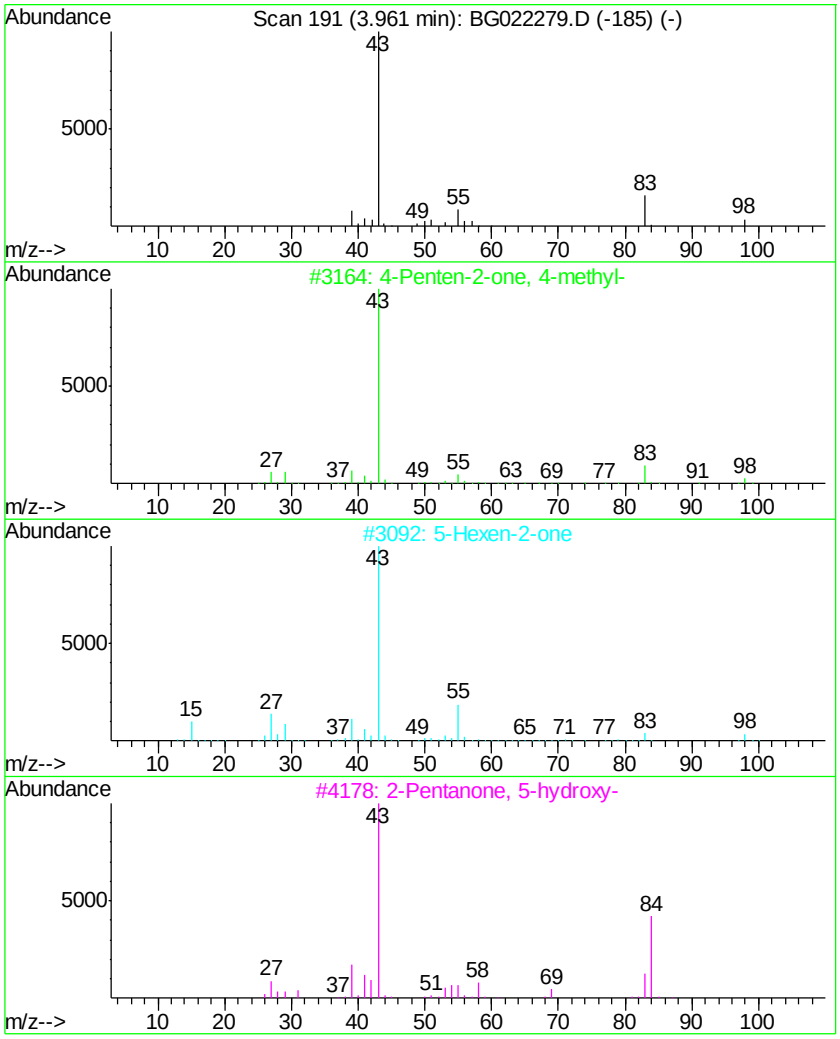
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

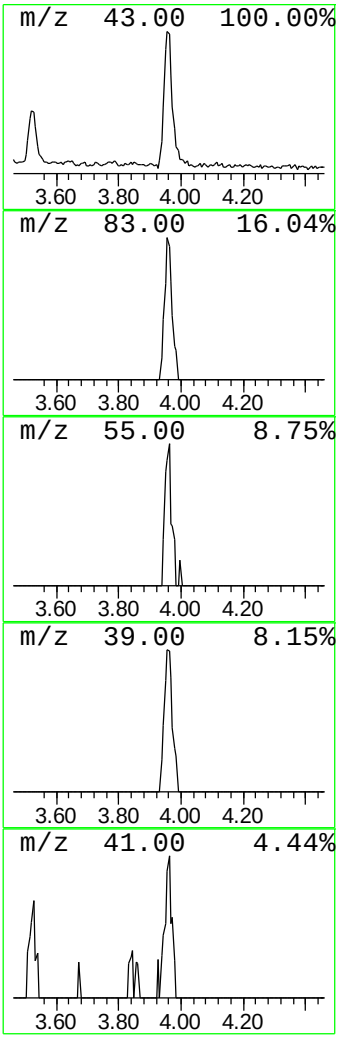
****

Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.96	3.45 ng	31976	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	58
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	2-Pentanone, 5-hydroxy-	102	C5H10O2	001071-73-4	9
4	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	9
5	2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG060916\
Data File : BG022279.D
Acq On : 10 Jun 2016 4:31
Operator : UM/SJ
Sample : H3396-04
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : STA-942-PLATFORM(0-4)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

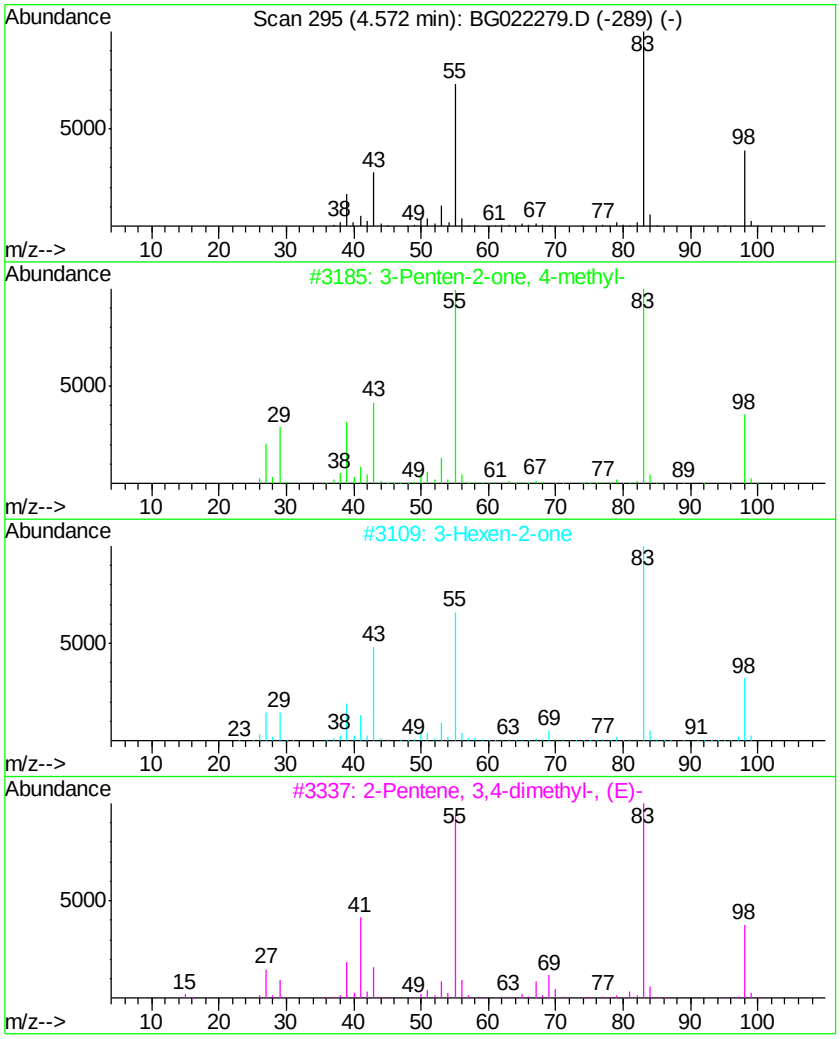
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

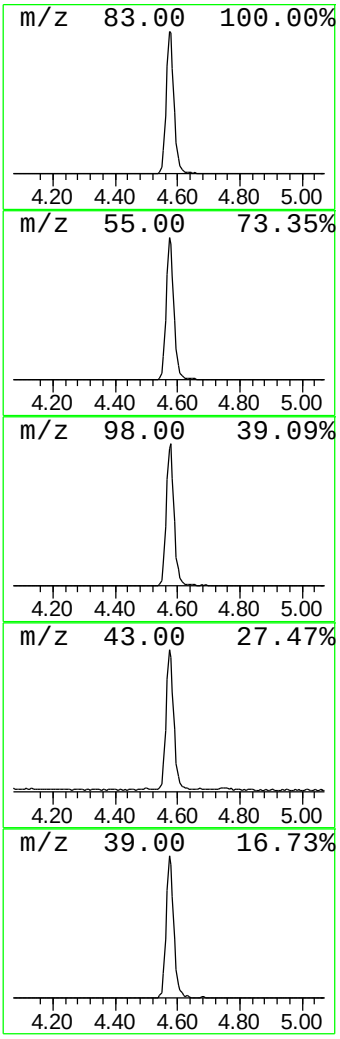
****

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.57	68.84 ng	637506	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4	Cyclohexane, methyl-	98	C7H14	000108-87-2	80
5	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG060916\
Data File : BG022279.D
Acq On : 10 Jun 2016 4:31
Operator : UM/SJ
Sample : H3396-04
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
STA-942-PLATFORM(0-4)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

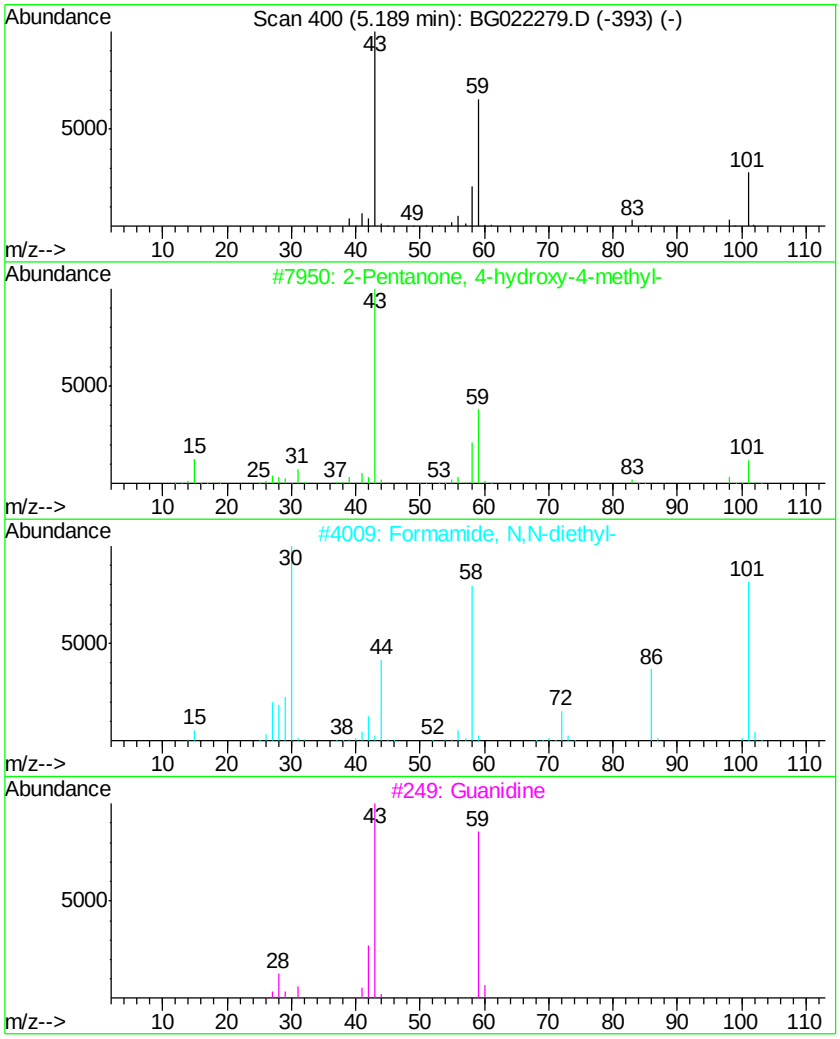
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

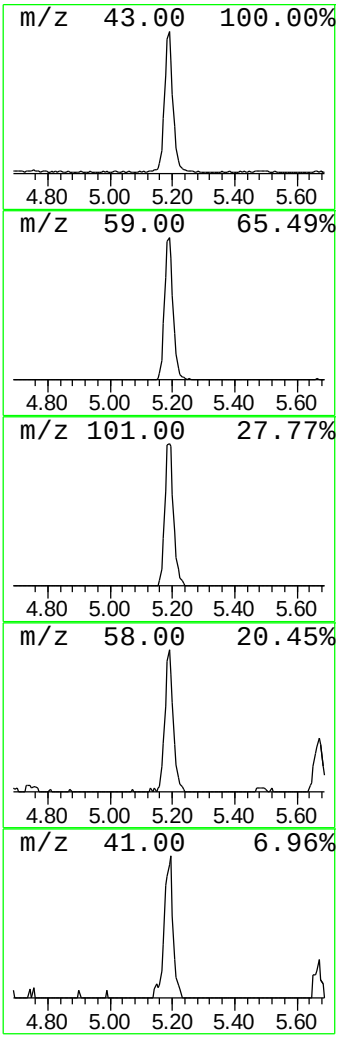
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	18.36 ng	170023	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9
3	Guanidine	59	CH5N3	000113-00-8	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG060916\
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Acq On : 10 Jun 2016 4:31
Operator : UM/SJ
Sample : H3396-04
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : STA-942-PLATFORM(0-4)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

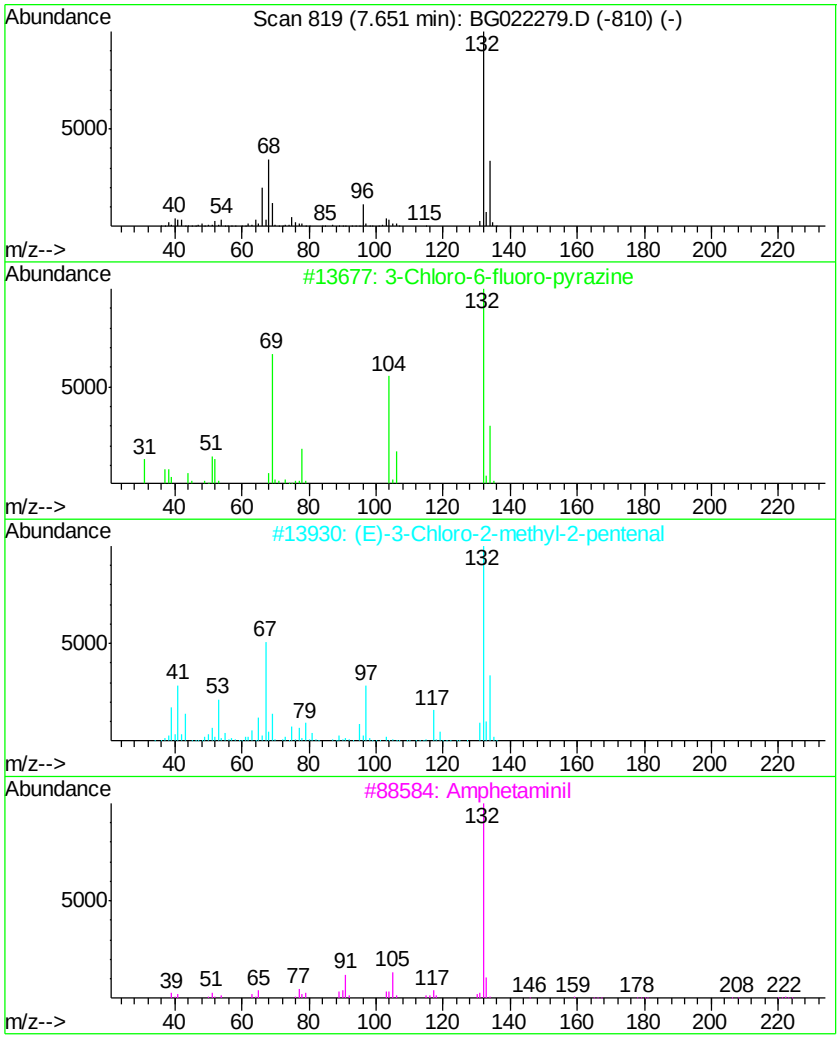
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

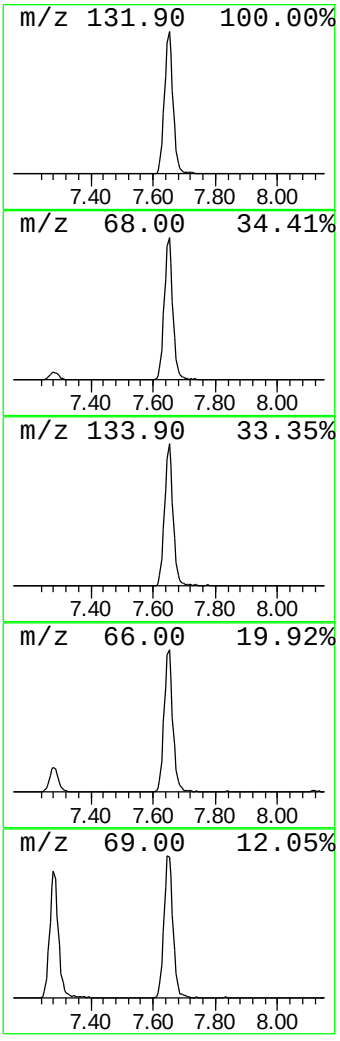
****

Peak Number 5 unknown7.65 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	113.22 ng	1048520	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Amphetaminil	250	C17H18N2	017590-01-1	12
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

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Instrument : BNA_G
ClientSampleId : STA-942-PLATFORM(0-4)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

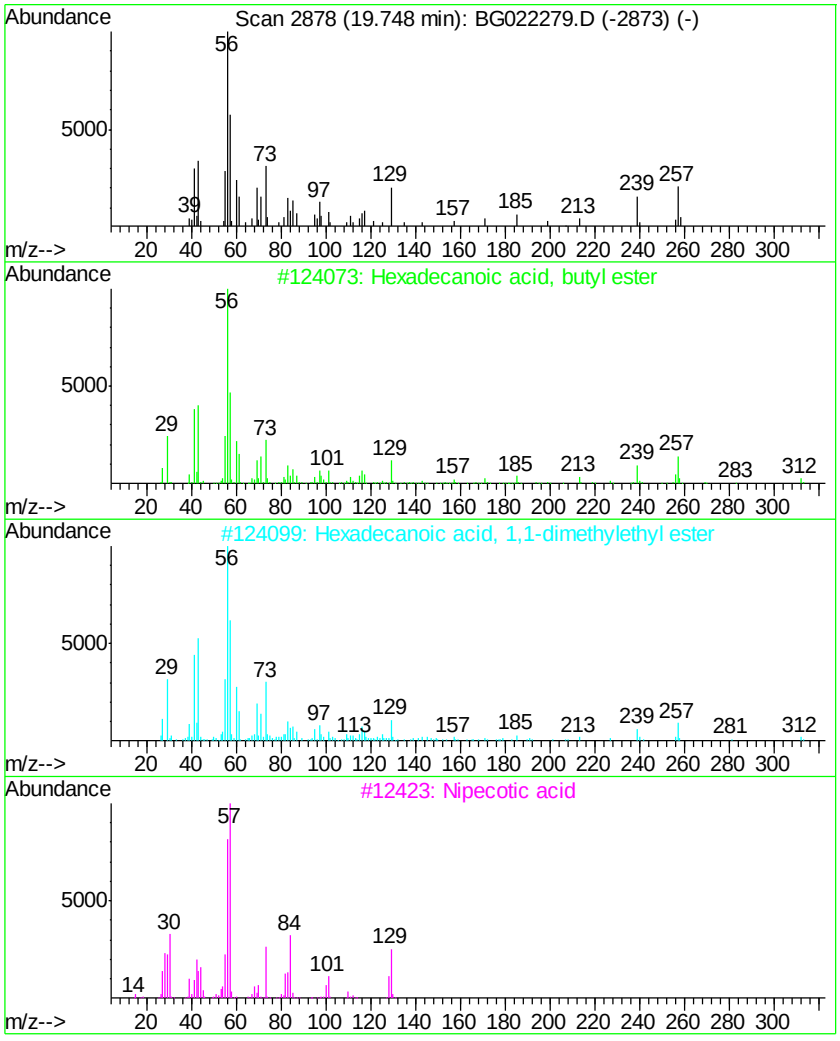
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

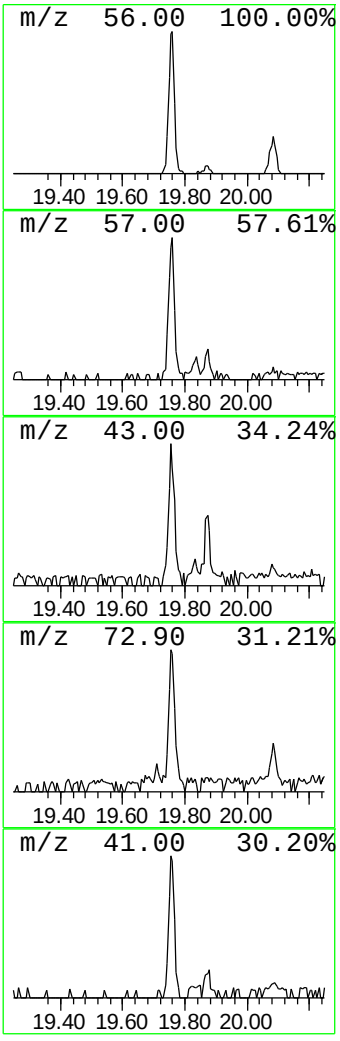
****

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.75	3.40 ng	82661	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	83
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	68
3	Nipecotic acid	129	C6H11NO2	000498-95-3	47
4	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	32
5	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	27





Data Path : Z:\HPCHEM1\BNA G\DATA\BG060916\
Data File : BG022279.D
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Operator : UM/SJ
Sample : H3396-04
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : STA-942-PLATFORM(0-4)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

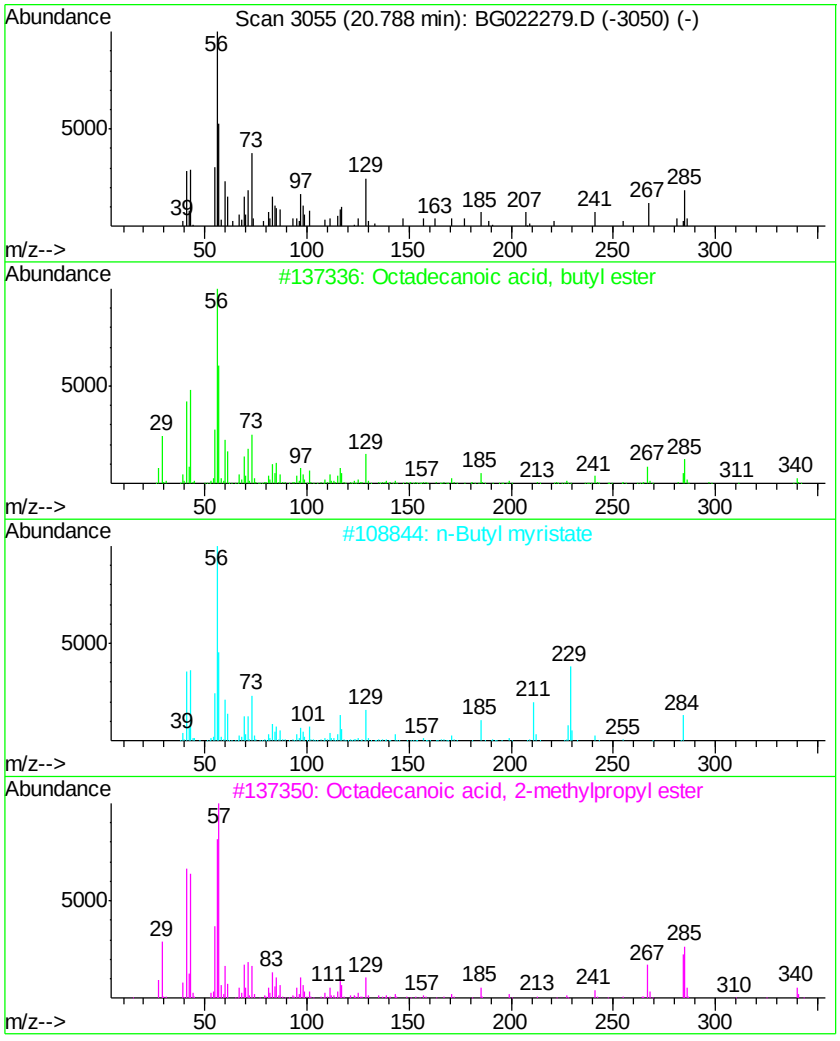
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

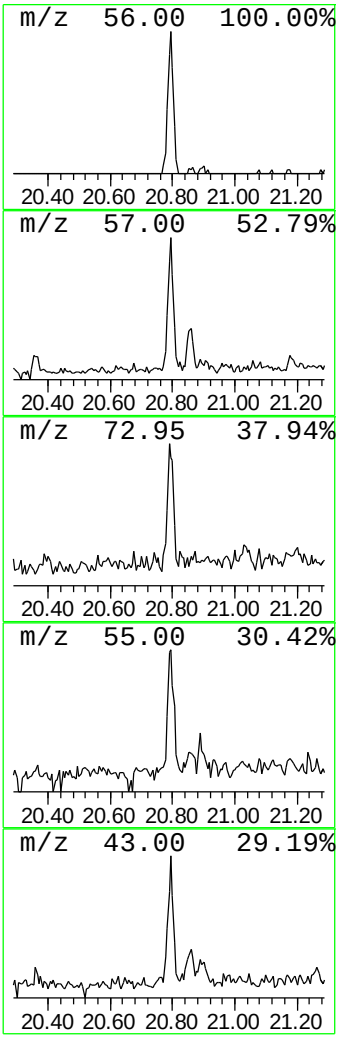
****

Peak Number 8 Octadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.79	2.45 ng	59515	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	93
2	n-Butyl myristate	284	C18H36O2	000110-36-1	50
3	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	38
4	2-Methyl-1-octadecene	266	C19H38	061868-20-0	27
5	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060916\
Data File : BG022279.D
Acq On : 10 Jun 2016 4:31
Operator : UM/SJ
Sample : H3396-04
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
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
Acetic acid	2.87	163.1	ng	1510180	1	8.11	185221	20.0
4-Penten-2-one, 4...	3.96	3.5	ng	31976	1	8.11	185221	20.0
3-Penten-2-one, 4...	4.57	68.8	ng	637506	1	8.11	185221	20.0
2-Pentanone, 4-hy...	5.19	18.4	ng	170023	1	8.11	185221	20.0
unknown7.65	7.65	113.2	ng	1048520	1	8.11	185221	20.0
Hexadecanoic acid...	19.75	3.4	ng	82661	5	21.77	486115	20.0
Octadecanoic acid...	20.79	2.5	ng	59515	5	21.77	486115	20.0