LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019898.D
Acq On : 4 Dec 2015 8:55
Operator : UM/NP
Sample : G4609-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-5-14.5-15.0-113015

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-BG120215.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	2.997	23	27	35	rVB	27776	38384	2.01%	0.354%
2	3.138	46	51	61	rBV	40024	76859	4.02%	0.708%
3	3.220	61	65	75	rVB	56164	80579	4.21%	0.742%
4	5.194	395	401	410	rVB	78459	120585	6.30%	1.111%
5	5.658	473	480	487	rBV	366011	571919	29.90%	5.267%
6	7.262	745	753	763	rBV	404391	683291	35.72%	6.293%
7	7.644	811	818	827	rBV	385013	638173	33.36%	5.877%
8	8.120	892	899	905	rBV	102148	165135	8.63%	1.521%
9	8.443	947	954	962	rVB	271159	464784	24.30%	4.280%
10	9.283	1090	1097	1106	rVB	246221	431383	22.55%	3.973%
11	10.934	1371	1378	1387	rVB	141325	253317	13.24%	2.333%
12	13.379	1786	1794	1804	rBV	713392	1130435	59.10%	10.411%
13	14.195	1927	1933	1939	rBV	173143	245480	12.83%	2.261%
14	14.748	2020	2027	2034	rVB2	260521	408718	21.37%	3.764%
15	15.588	2166	2170	2174	rVB	16158	20731	1.08%	0.191%
16	16.228	2272	2279	2287	rBV	661316	979426	51.20%	9.020%
17	16.446	2312	2316	2319	rBV	18569	25723	1.34%	0.237%
18	17.239	2445	2451	2455	rBV3	13706	20317	1.06%	0.187%
19	17.491	2487	2494	2500	rBV2	358906	543723	28.43%	5.007%
20	18.367	2639	2643	2650	rBV2	36438	55840	2.92%	0.514%
21	19.225	2786	2789	2794	rBV4	14850	20509	1.07%	0.189%
22	19.548	2837	2844	2848	rBV2	15638	23996	1.25%	0.221%
23	19.636	2855	2859	2865	rBV8	12267	21611	1.13%	0.199%
24	19.771	2878	2882	2889	rBV2	16973	26812	1.40%	0.247%
25	20.094	2931	2937	2942	rBV	1456851	1912829	100.00%	17.616%
26	20.300	2968	2972	2977	rBV	26249	33121	1.73%	0.305%
27	20.782	3050	3054	3060	rVB	45996	60876	3.18%	0.561%
28	20.858	3062	3067	3073	rVB4	26440	46144	2.41%	0.425%
29	20.993	3087	3090	3095	rBV2	28822	45877	2.40%	0.423%
30	21.046	3095	3099	3103	rVB	56276	68070	3.56%	0.627%
31	21.117	3108	3111	3119	rVB3	24191	34285	1.79%	0.316%
32	21.404	3156	3160	3167	rVB4	32485	46706	2.44%	0.430%
33	21.557	3183	3186	3191	rVB	43747	56448	2.95%	0.520%
34	21.628	3195	3198	3202	rBV5	22087	36664	1.92%	0.338%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019898.D
Acq On : 4 Dec 2015 8:55
Operator : UM/NP
Sample : G4609-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-5-14.5-15.0-113015

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-BG120215.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	21.763	3215	3221	3230	rVB	416687	700329	36.61%	6.450%
36	22.110	3278	3280	3285	rVB2	18754	26832	1.40%	0.247%
37	22.738	3383	3387	3394	rVB3	15228	26925	1.41%	0.248%
38	23.091	3444	3447	3451	rVB5	14796	21158	1.11%	0.195%
39	23.514	3513	3519	3525	rBV	37916	73083	3.82%	0.673%
40	25.053	3771	3781	3791	rBV	222998	621193	32.48%	5.721%

Sum of corrected areas: 10858270

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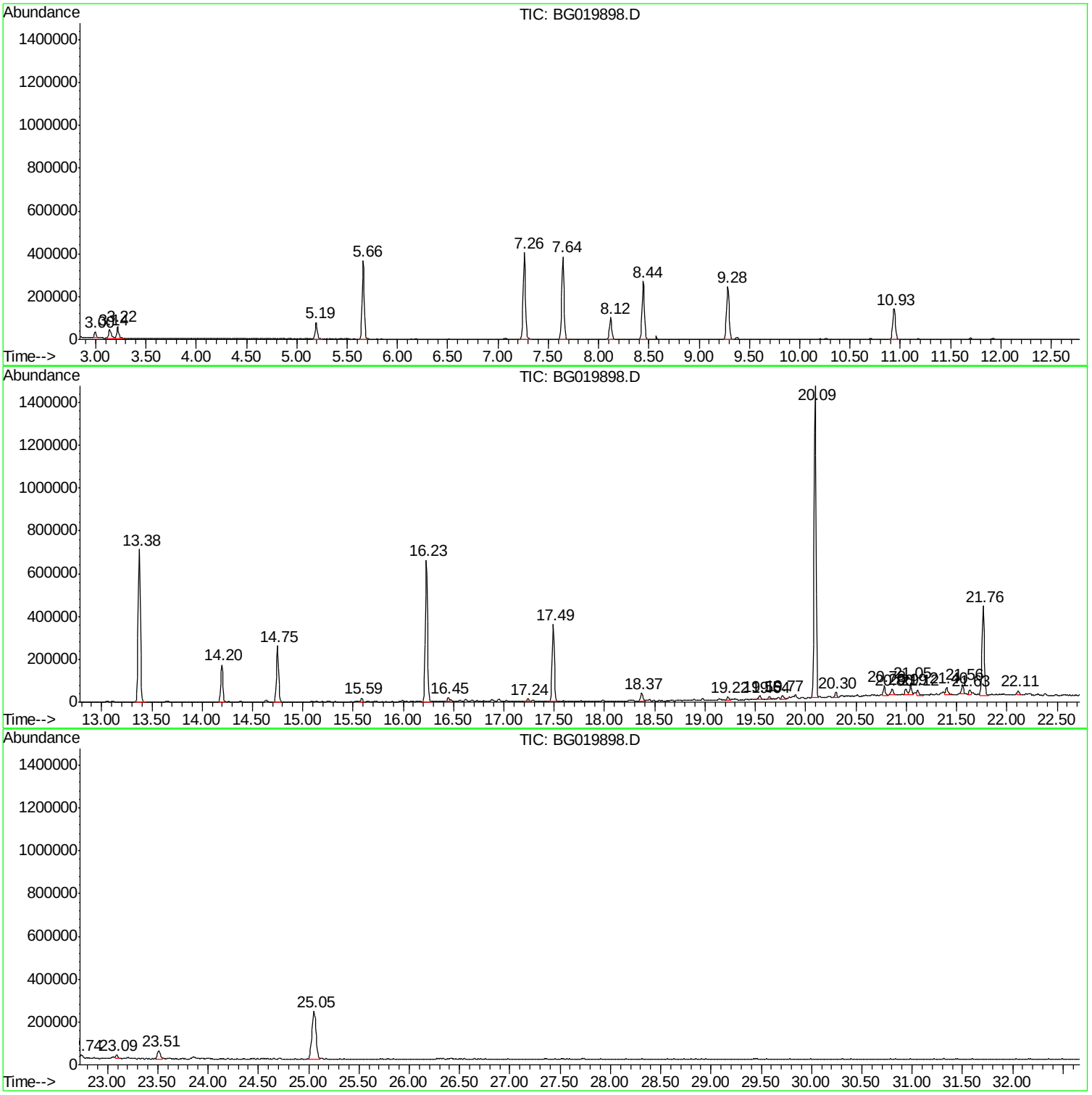
Data File : BG019898.D
Acq On : 4 Dec 2015 8:55
Operator : UM/NP
Sample : G4609-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-5-14.5-15.0-113015

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019898.D
Acq On : 4 Dec 2015 8:55
Operator : UM/NP
Sample : G4609-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-5-14.5-15.0-113015

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

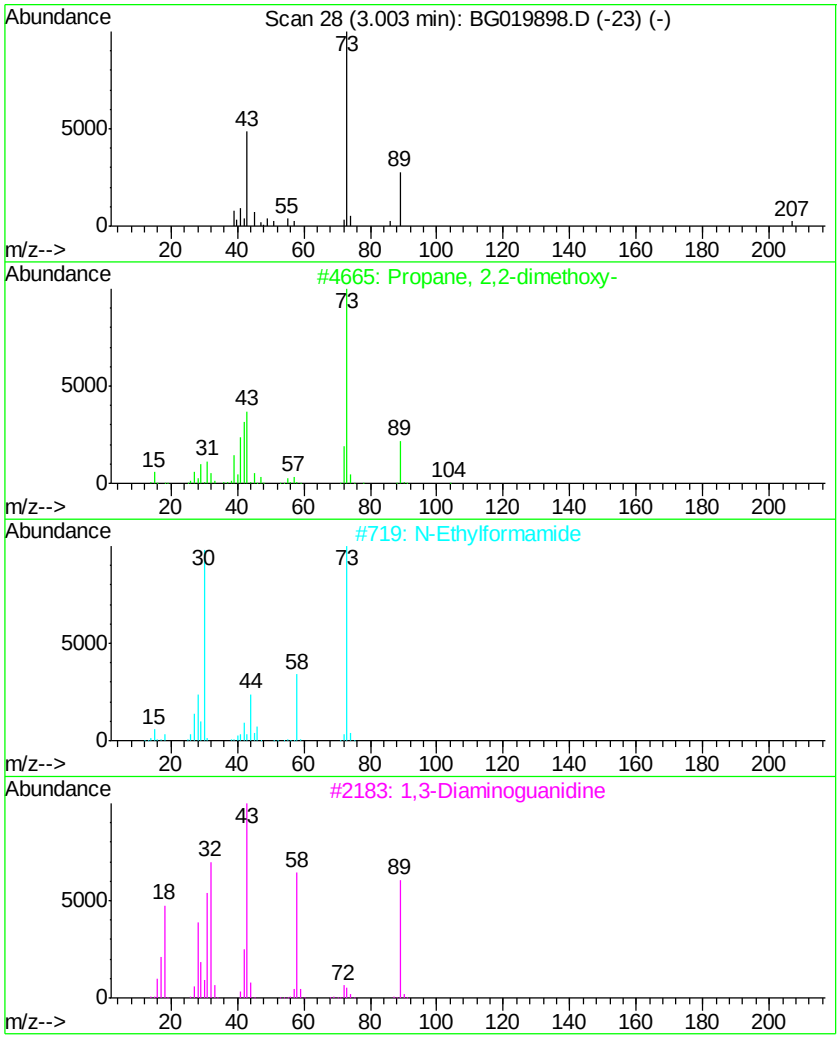
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

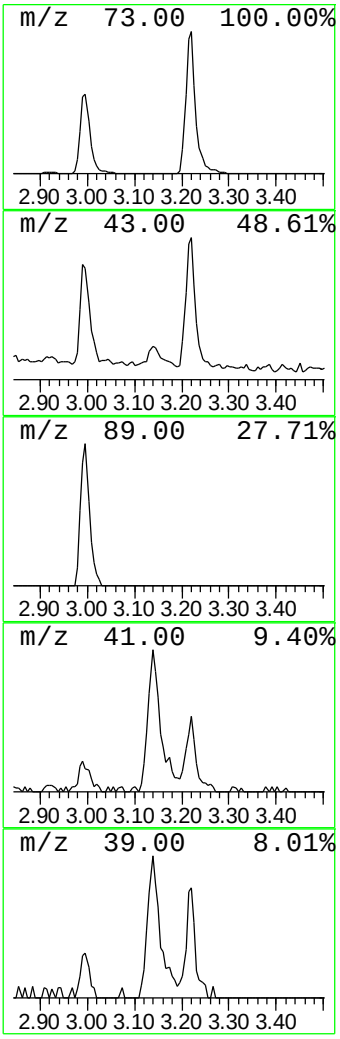
****

Peak Number 1 unknown3.00 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.00	4.65 ng	38384	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	45
2	N-Ethylformamide	73	C3H7NO	000627-45-2	16
3	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019898.D
Acq On : 4 Dec 2015 8:55
Operator : UM/NP
Sample : G4609-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-5-14.5-15.0-113015

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.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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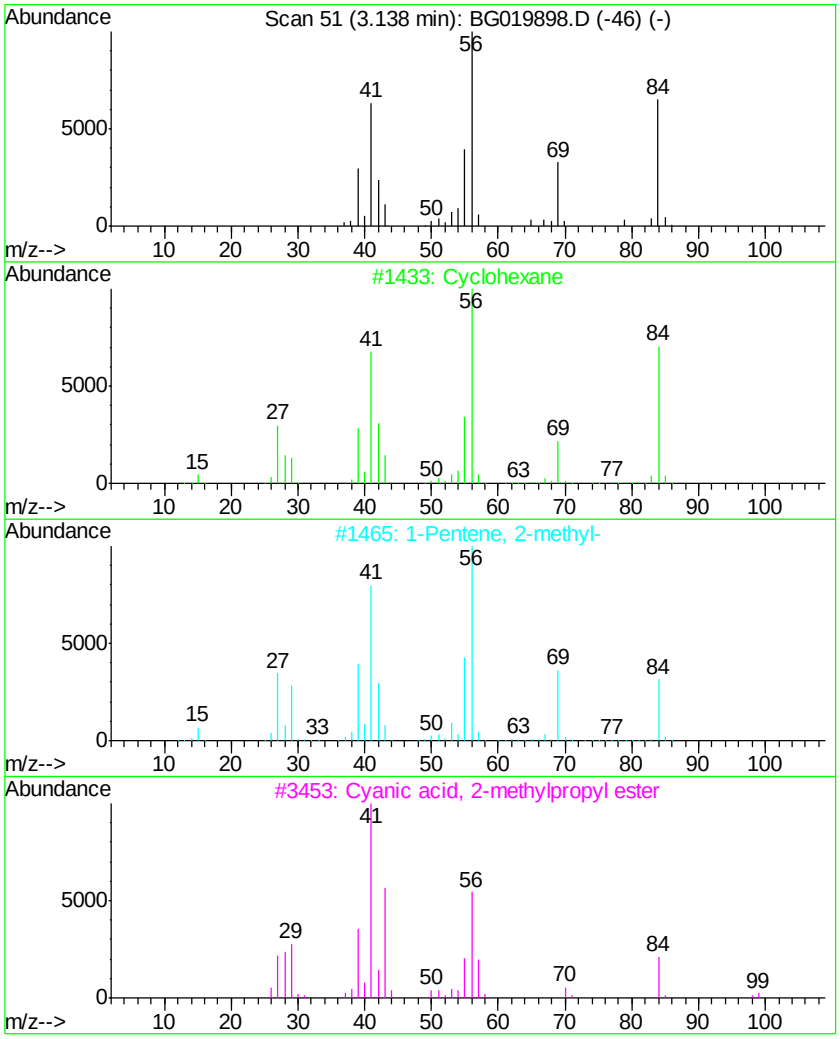
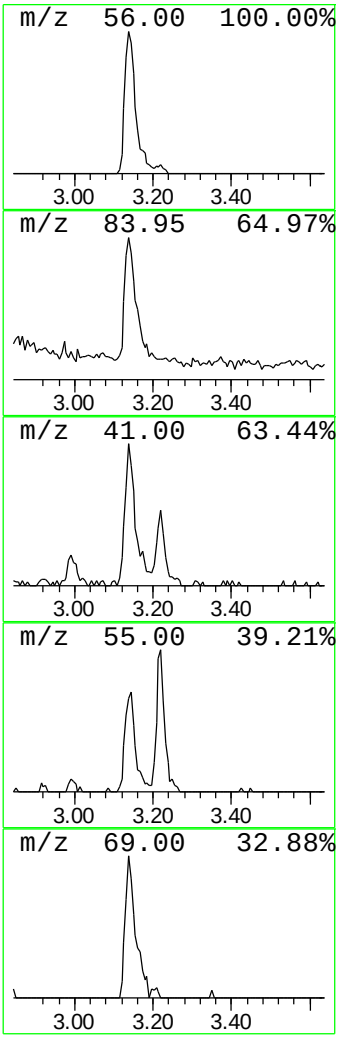
Peak Number 2 Cyclohexane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.14	9.31 ng	76859	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	91
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	80
3	Cyanic acid, 2-methylpropyl ester	99	C5H9NO	001768-25-8	64
4	Cyclopentane, methyl-	84	C6H12	000096-37-7	59
5	1-Hexene	84	C6H12	000592-41-6	53





Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019898.D
Acq On : 4 Dec 2015 8:55
Operator : UM/NP
Sample : G4609-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-5-14.5-15.0-113015

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.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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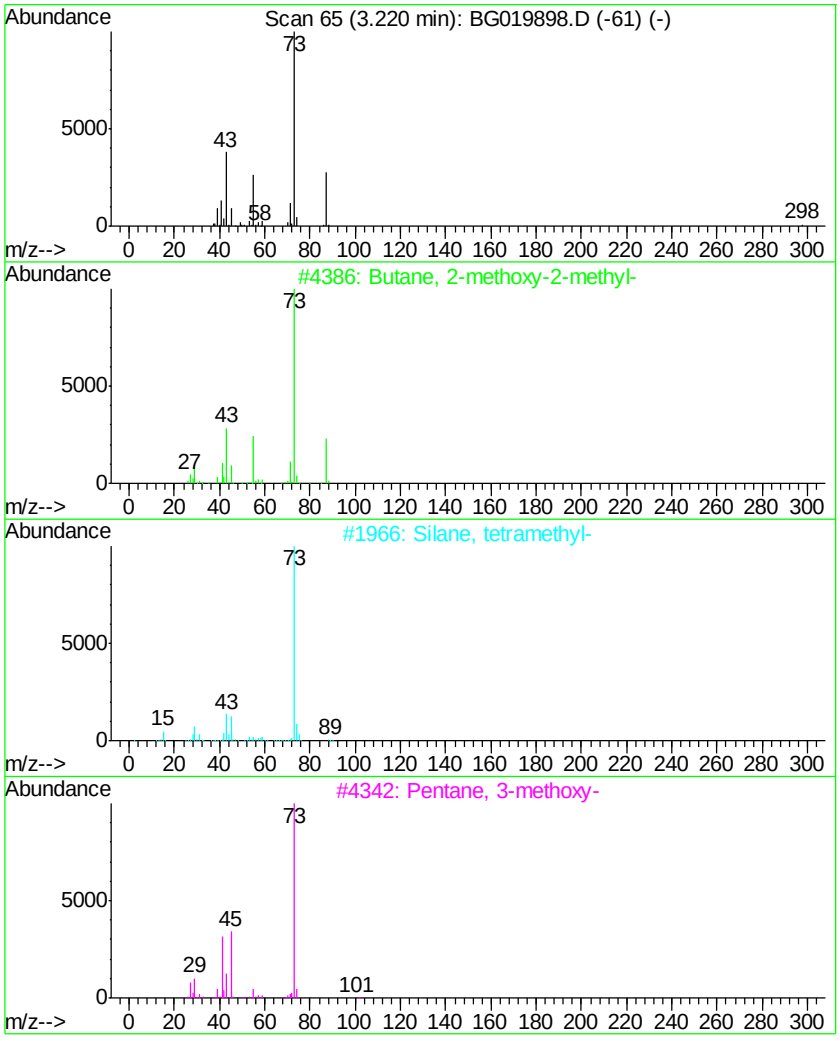
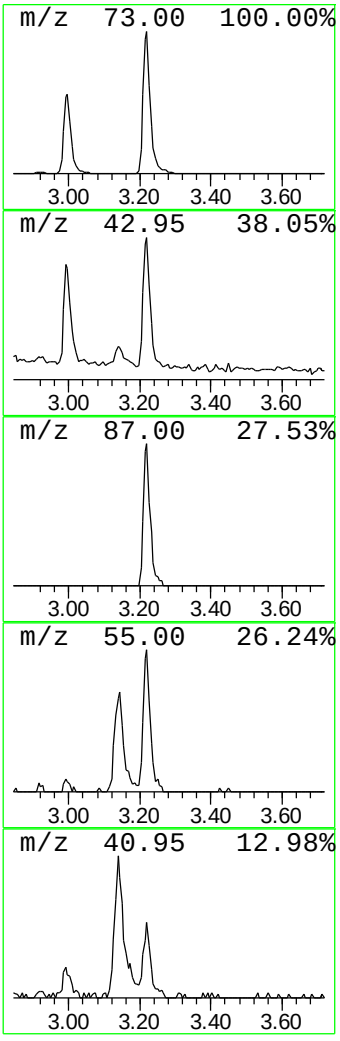
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.22	9.76 ng	80579	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019898.D
Acq On : 4 Dec 2015 8:55
Operator : UM/NP
Sample : G4609-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-5-14.5-15.0-113015

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

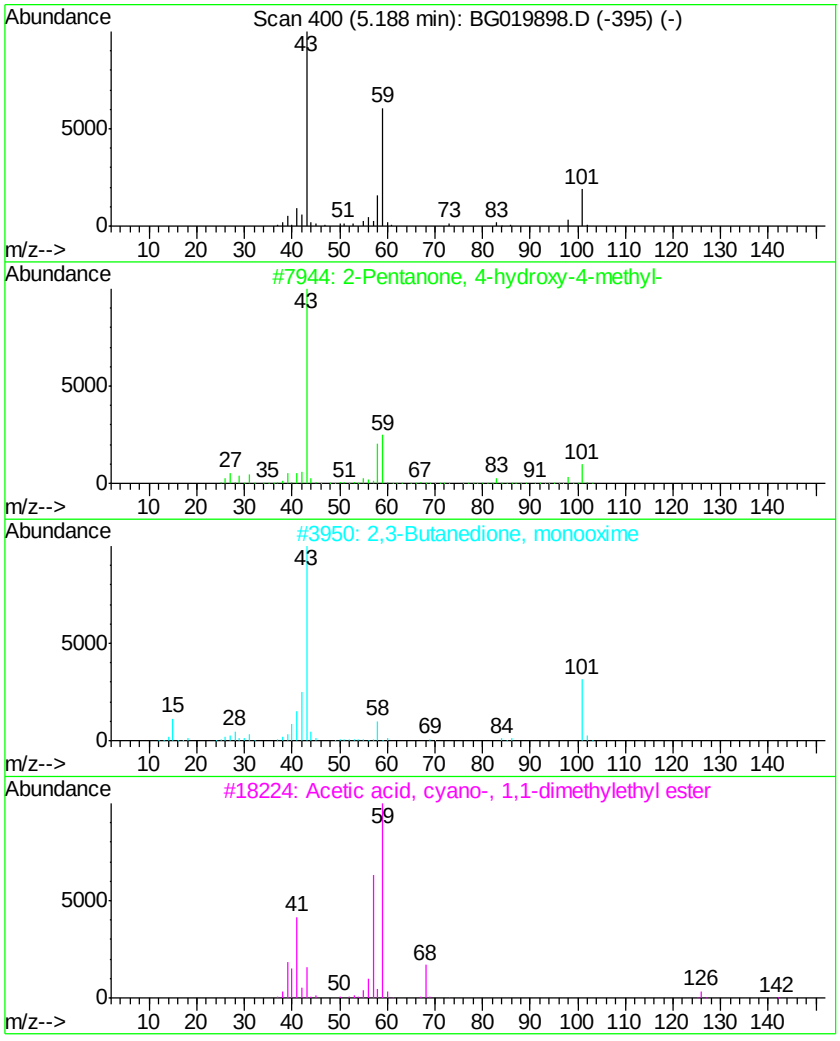
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

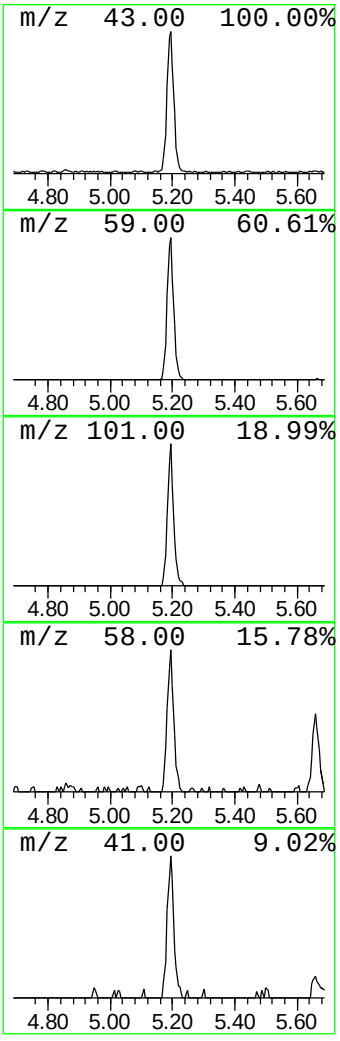
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	14.60 ng	120585	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	2-Nonanone	142	C9H18O	000821-55-6	12
5	Acetone	58	C3H6O	000067-64-1	10





Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019898.D
Acq On : 4 Dec 2015 8:55
Operator : UM/NP
Sample : G4609-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-5-14.5-15.0-113015

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

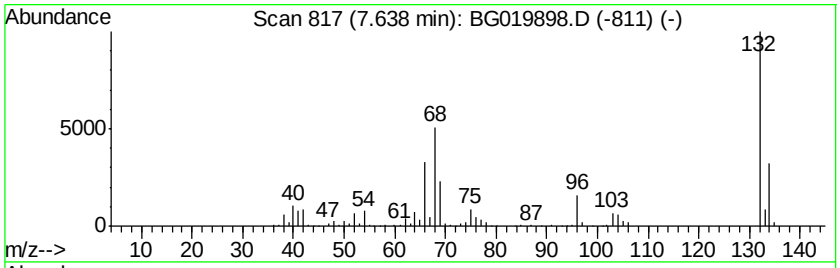
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

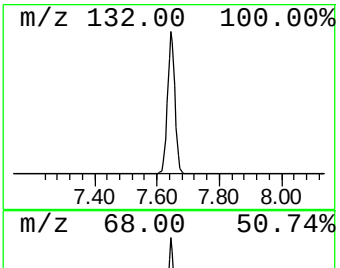
****

Peak Number 5 unknown7.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	77.29 ng	638173	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
2	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





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Acq On : 4 Dec 2015 8:55
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Sample : G4609-03
Misc :
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Instrument : BNA_G
ClientSampleId : SB-5-14.5-15.0-113015

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

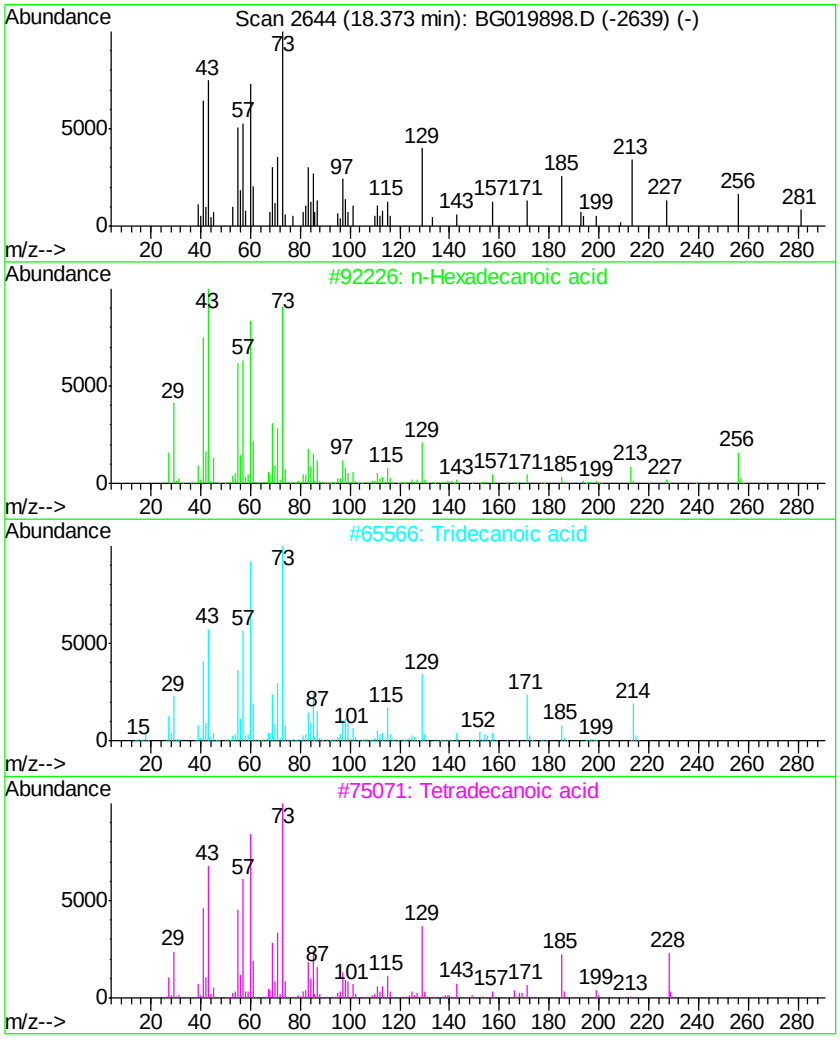
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

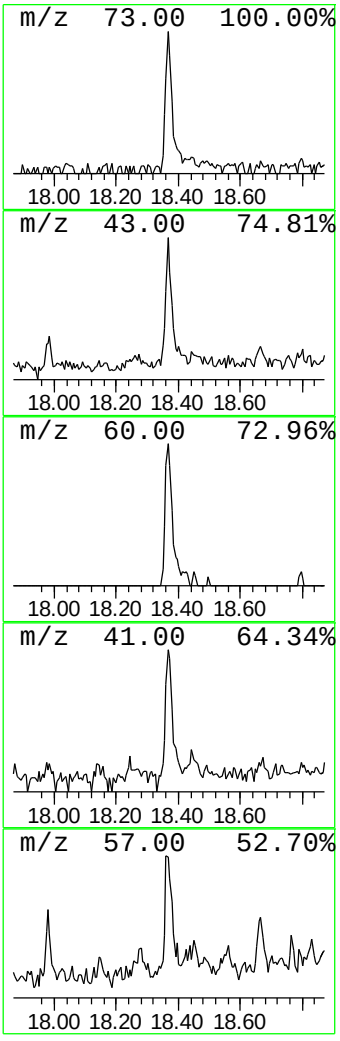
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.37	2.05 ng	55840	Phenanthrene-d10	17.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
2	Tridecanoic acid	214	C13H26O2	000638-53-9	50
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
4	Undecanoic acid	186	C11H22O2	000112-37-8	47
5	Dodecanoic acid	200	C12H24O2	000143-07-7	43





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Data File : BG019898.D
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Operator : UM/NP
Sample : G4609-03
Misc :
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Instrument : BNA_G
ClientSampleId : SB-5-14.5-15.0-113015

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.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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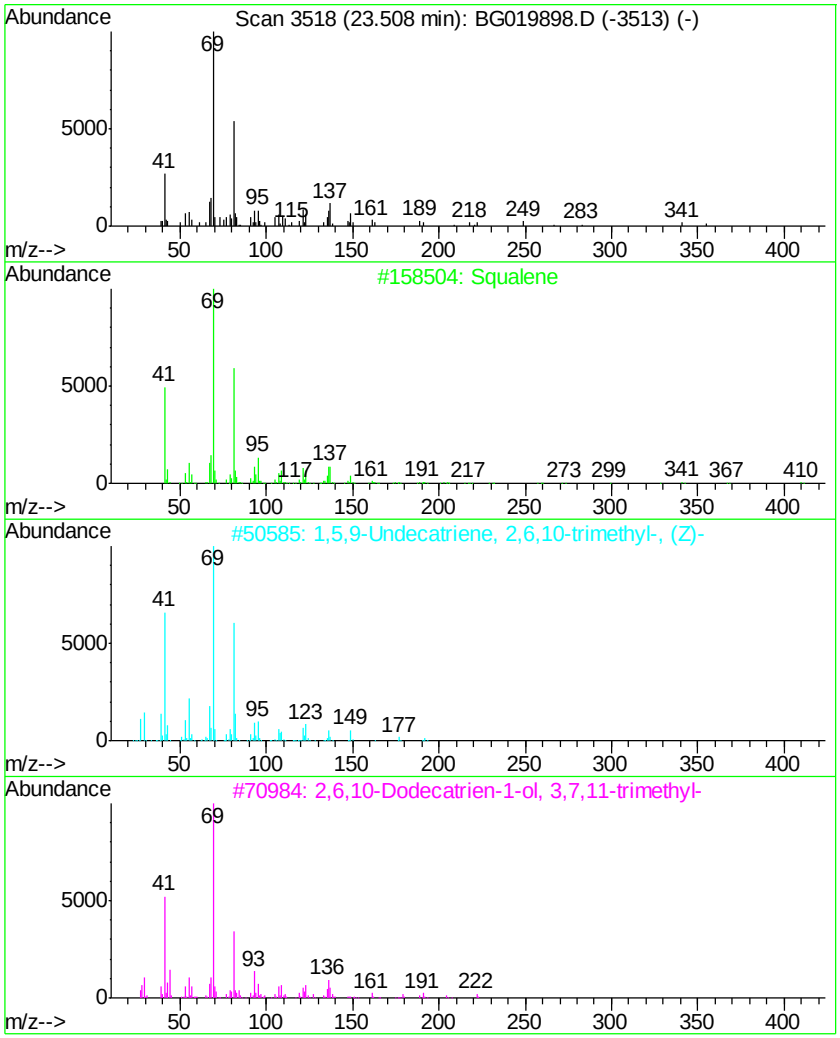
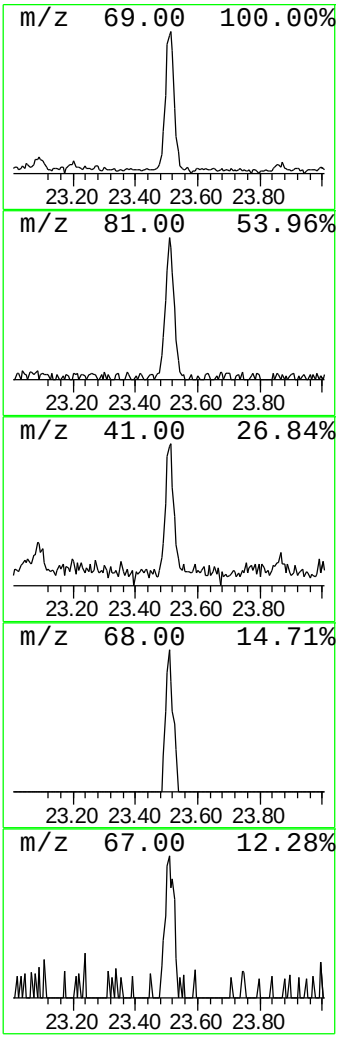
Peak Number 8 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.51	2.35 ng	73083	Perylene-d12	25.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	87
2	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	83
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	80
4	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	78
5	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG120315\
Data File : BG019898.D
Acq On : 4 Dec 2015 8:55
Operator : UM/NP
Sample : G4609-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-5-14.5-15.0-113015

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.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
unknown3.00	3.00	4.7	ng	38384	1	8.12	165135	20.0
Cyclohexane	3.14	9.3	ng	76859	1	8.12	165135	20.0
Butane, 2-methoxy...	3.22	9.8	ng	80579	1	8.12	165135	20.0
2-Pentanone, 4-hy...	5.19	14.6	ng	120585	1	8.12	165135	20.0
unknown7.64	7.64	77.3	ng	638173	1	8.12	165135	20.0
n-Hexadecanoic acid	18.37	2.0	ng	55840	4	17.49	543723	20.0
Squalene	23.51	2.4	ng	73083	6	25.05	621193	20.0