LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093647.D
Acq On : 14 Mar 2017 9:52
Operator : SJ/MA
Sample : I2201-23
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-126

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-BF030717.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	2.436	43	48	60	rBV	44254	152369	2.86%	0.334%
2	3.144	108	110	125	rBV	36329	137108	2.57%	0.300%
3	4.173	198	200	218	rVB	509593	1047090	19.62%	2.294%
4	4.870	259	261	280	rBV	894266	1697390	31.81%	3.718%
5	5.316	298	300	333	rBV	3503580	5306799	99.45%	11.625%
6	5.727	333	336	350	rVB	37166	106857	2.00%	0.234%
7	6.367	391	392	400	rBV	2822504	4962231	93.00%	10.870%
8	6.482	400	402	405	rVB	4483592	4715233	88.37%	10.329%
9	6.710	420	422	430	rVB	1011414	998486	18.71%	2.187%
10	6.859	433	435	438	rBV	3276257	3763110	70.52%	8.244%
11	7.282	470	472	487	rBV	2520878	3501866	65.63%	7.671%
12	8.002	533	535	550	rVB	1229396	1340592	25.12%	2.937%
13	9.076	627	629	632	rBV	3983405	5335914	100.00%	11.689%
14	9.762	686	689	691	rBV	1027192	1395857	26.16%	3.058%
15	10.551	756	758	761	rBV2	2270994	2846591	53.35%	6.236%
16	11.248	817	819	826	rBV	1454712	1425662	26.72%	3.123%
17	12.654	940	942	944	rBV	184209	157604	2.95%	0.345%
18	12.837	955	958	960	rBV	4524641	4801395	89.98%	10.518%
19	13.362	1001	1004	1006	rBV	89074	99966	1.87%	0.219%
20	13.900	1049	1051	1062	rVB	743139	1100803	20.63%	2.411%
21	15.305	1171	1174	1188	rVB	398285	755789	14.16%	1.656%

Sum of corrected areas: 45648712

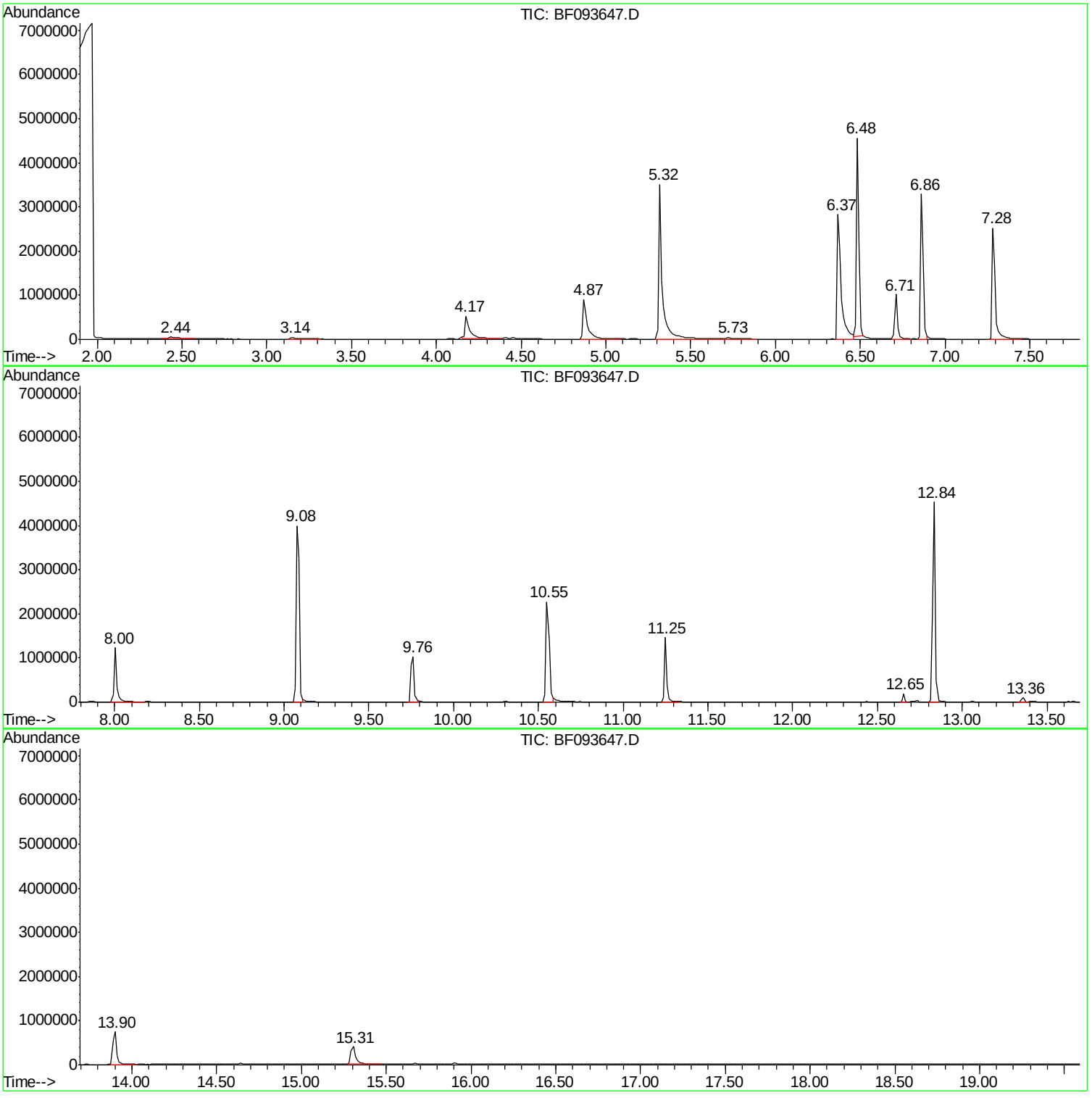
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093647.D
Acq On : 14 Mar 2017 9:52
Operator : SJ/MA
Sample : I2201-23
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-126

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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 F\DATA\BF031317\
Data File : BF093647.D
Acq On : 14 Mar 2017 9:52
Operator : SJ/MA
Sample : I2201-23
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-126

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

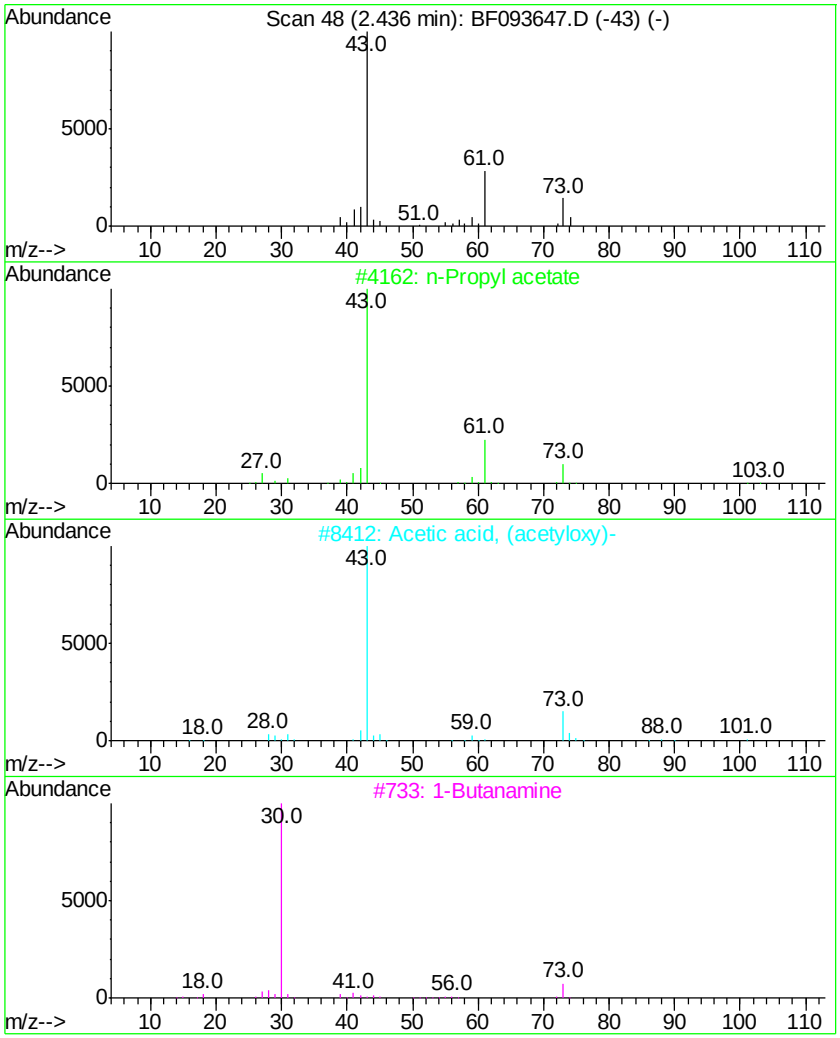
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

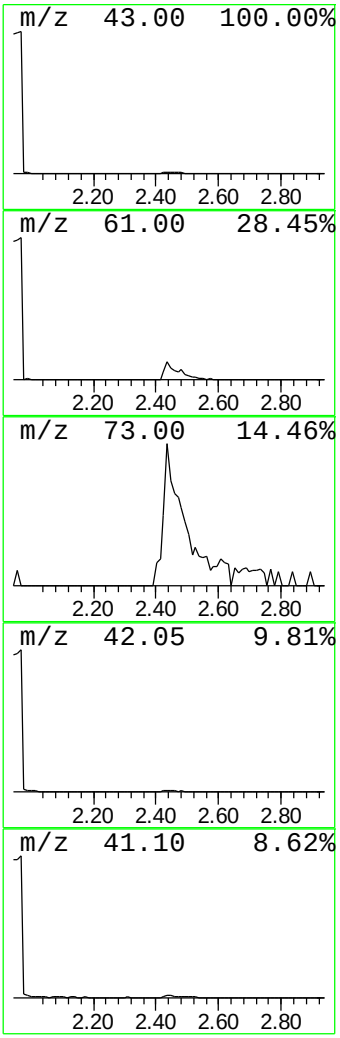
****

Peak Number 1 n-Propyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.44	3.05 ng	152369	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	64
2	Acetic acid, (acetyloxy)-	118	C4H6O4	013831-30-6	37
3	1-Butanamine	73	C4H11N	000109-73-9	9
4	Sulfurous acid, dipropyl ester	166	C6H14O3S	000623-98-3	9
5	Methanecarbothiolic acid	76	C2H4OS	000507-09-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093647.D
Acq On : 14 Mar 2017 9:52
Operator : SJ/MA
Sample : I2201-23
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-126

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

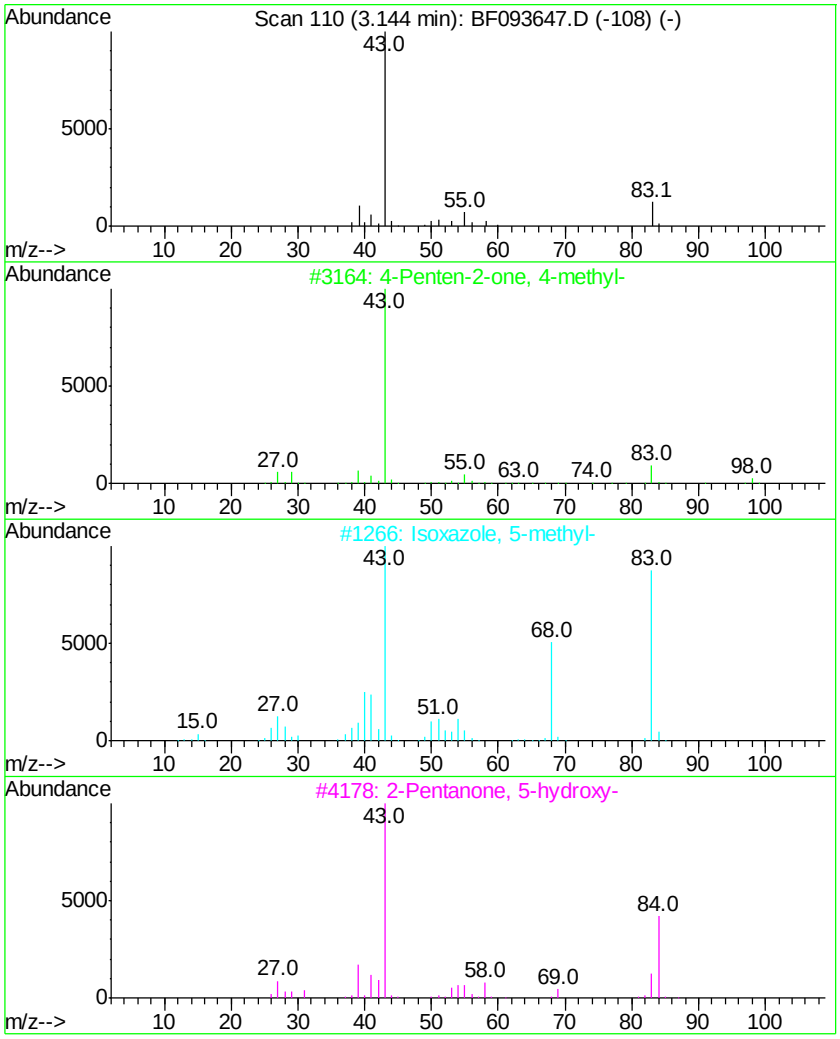
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

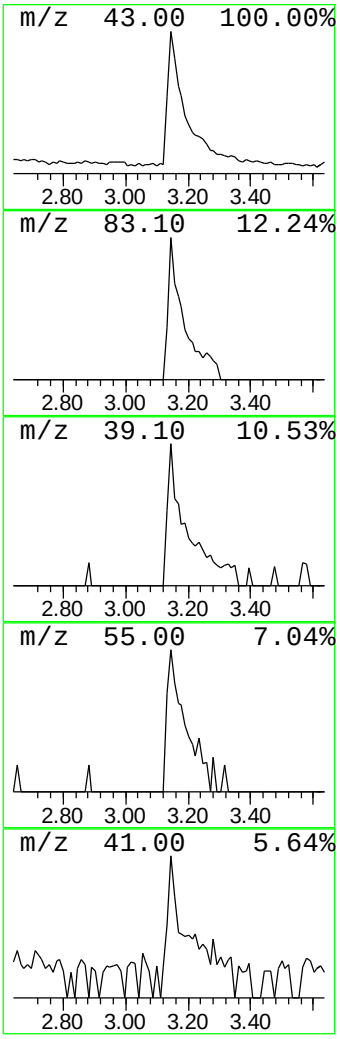
****

Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.14	2.75 ng	137108	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	64
2	Isoxazole, 5-methyl-	83	C4H5NO	005765-44-6	7
3	2-Pentanone, 5-hydroxy-	102	C5H10O2	001071-73-4	4
4	Isobutane	58	C4H10	000075-28-5	3
5	2-Butenenitrile, 4-acetoxy-, (Z+E)	125	C6H7NO2	1000158-79-0	2





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093647.D
Acq On : 14 Mar 2017 9:52
Operator : SJ/MA
Sample : I2201-23
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-126

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

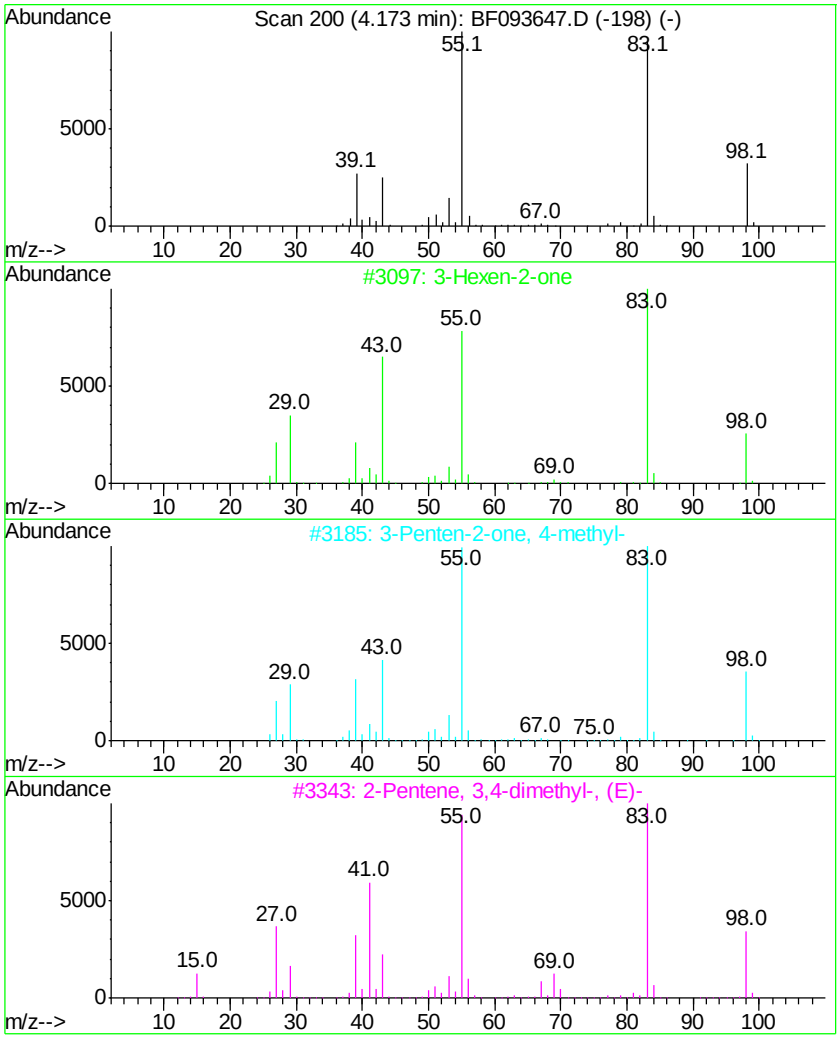
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

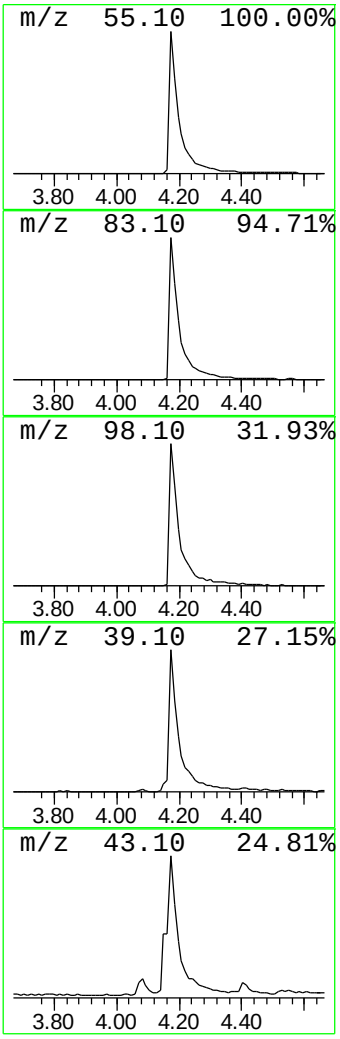
****

Peak Number 3 3-Hexen-2-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.17	20.97 ng	1047090	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	83
4	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	78
5	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093647.D
Acq On : 14 Mar 2017 9:52
Operator : SJ/MA
Sample : I2201-23
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-126

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

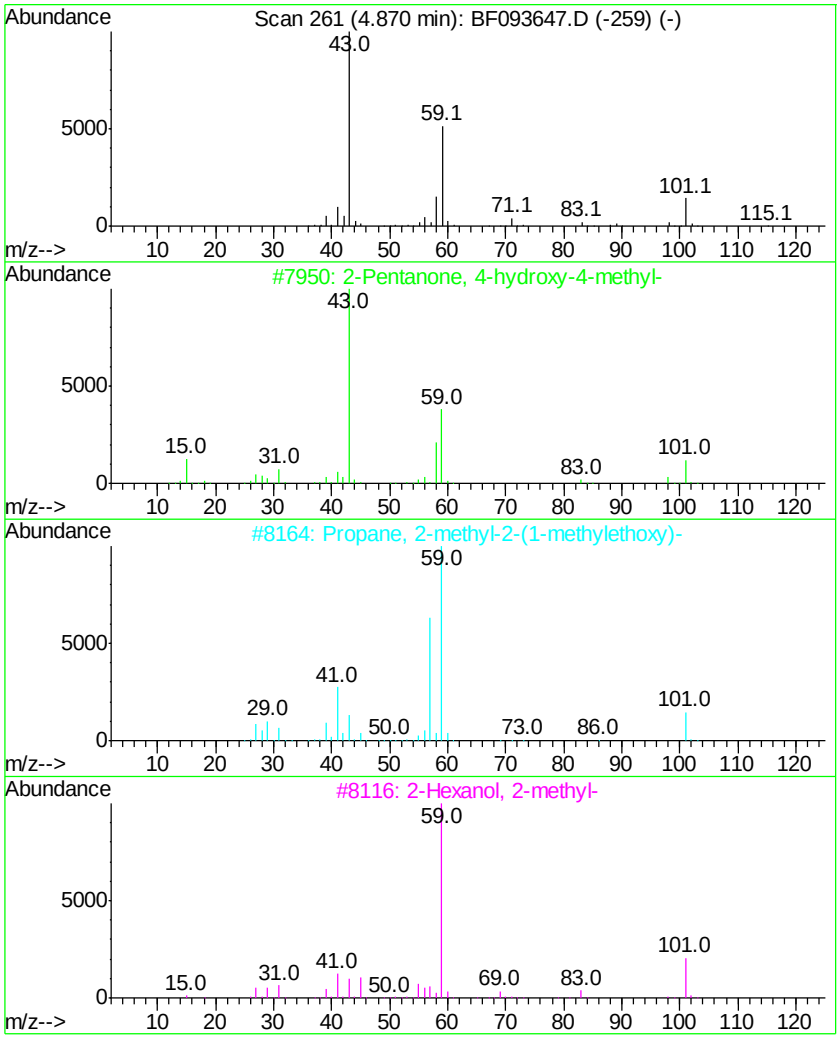
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

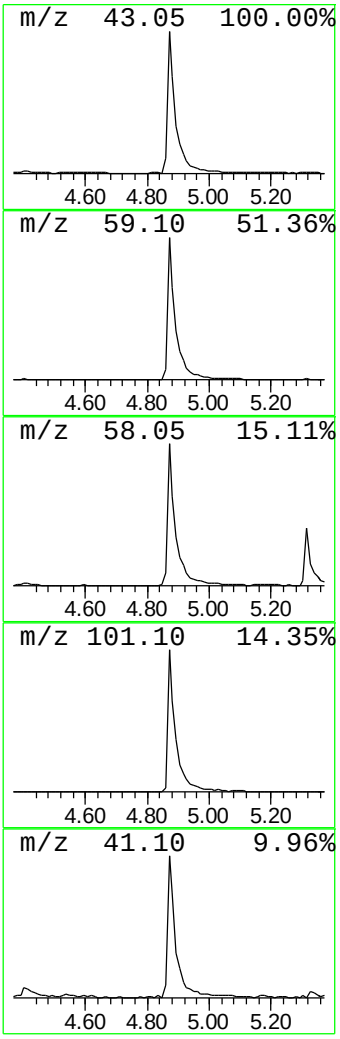
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	34.00 ng	1697390	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	23





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093647.D
Acq On : 14 Mar 2017 9:52
Operator : SJ/MA
Sample : I2201-23
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-126

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

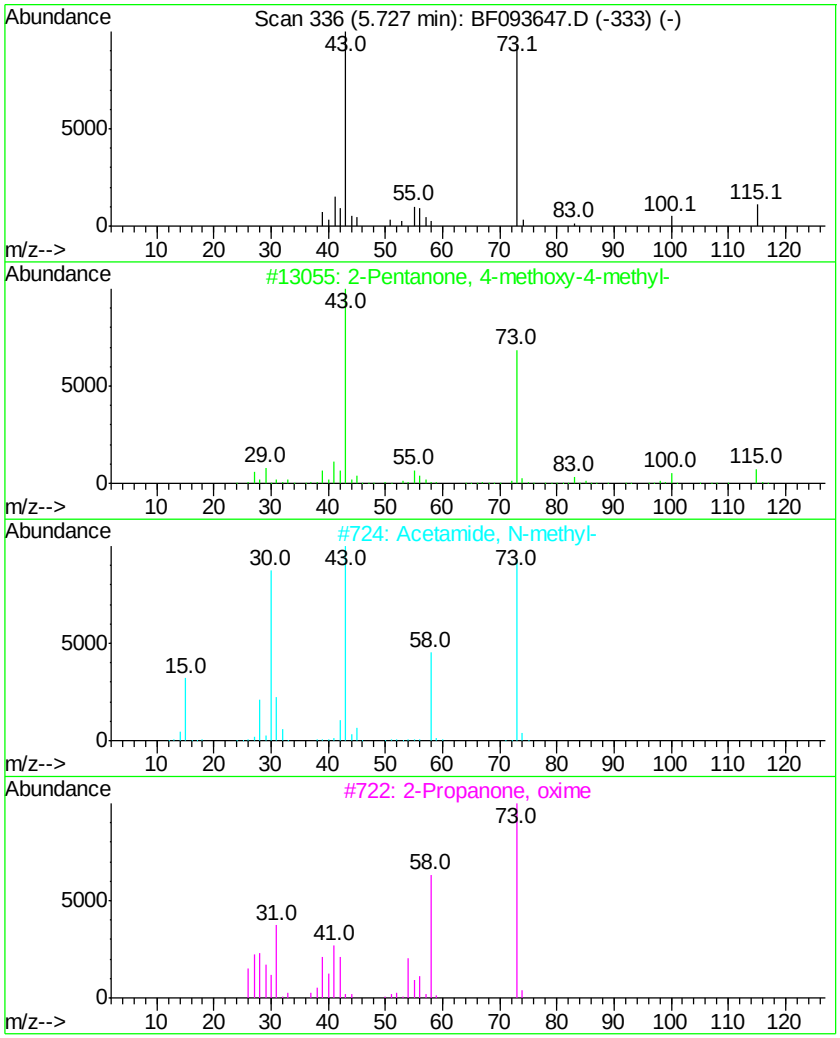
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

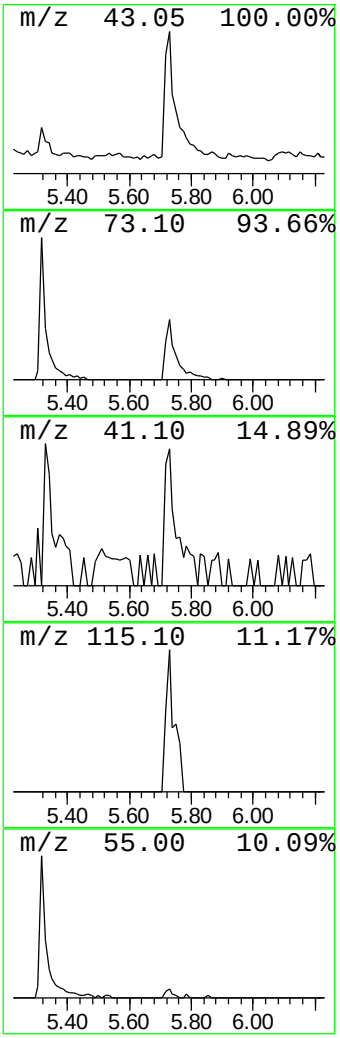
****

Peak Number 5 2-Pentanone, 4-methoxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.73	2.14 ng	106857	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	59
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	47
3	2-Propanone, oxime	73	C3H7NO	000127-06-0	9
4	N-Formylmorpholine	115	C5H9NO2	004394-85-8	9
5	Pentanal, 2-methyl-	100	C6H12O	000123-15-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093647.D
Acq On : 14 Mar 2017 9:52
Operator : SJ/MA
Sample : I2201-23
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-126

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

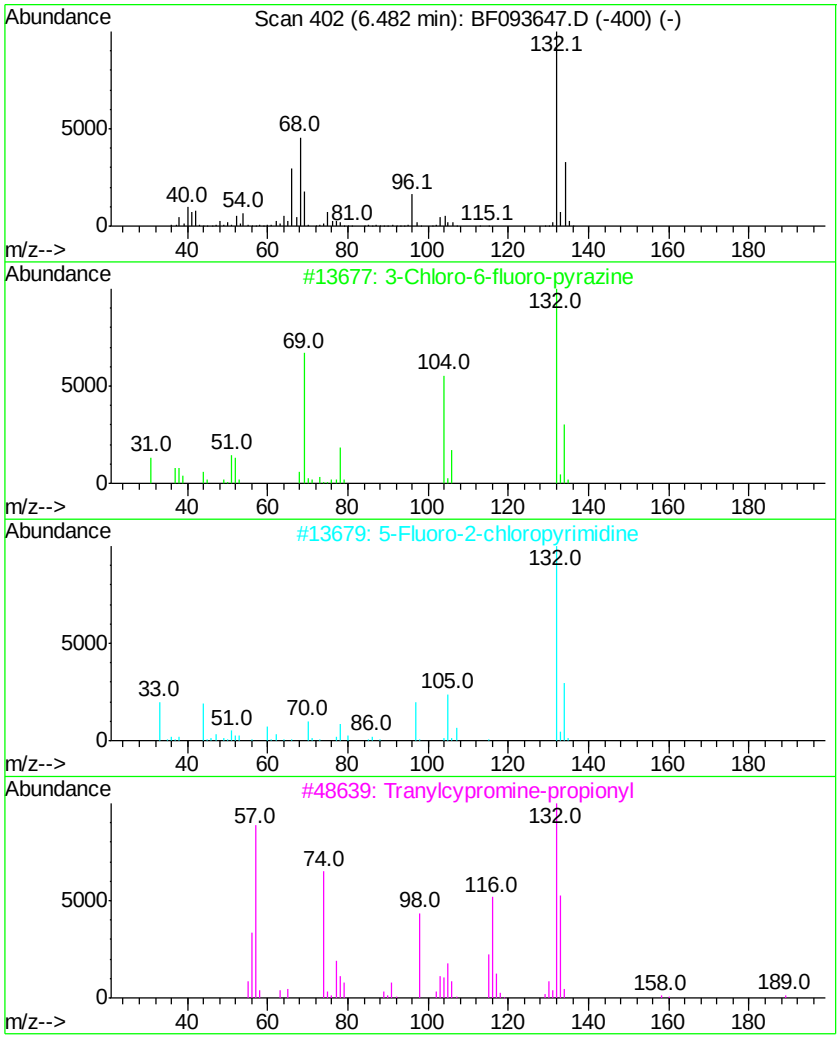
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

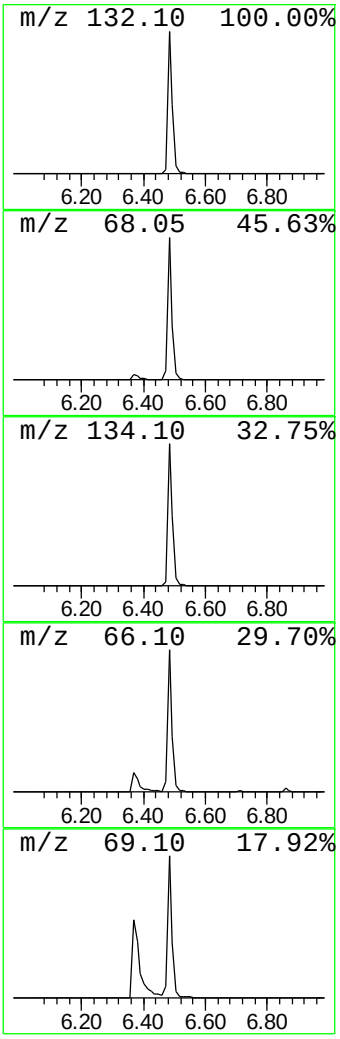
****

Peak Number 6 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	94.45 ng	4715230	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
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	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093647.D
Acq On : 14 Mar 2017 9:52
Operator : SJ/MA
Sample : I2201-23
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-126

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

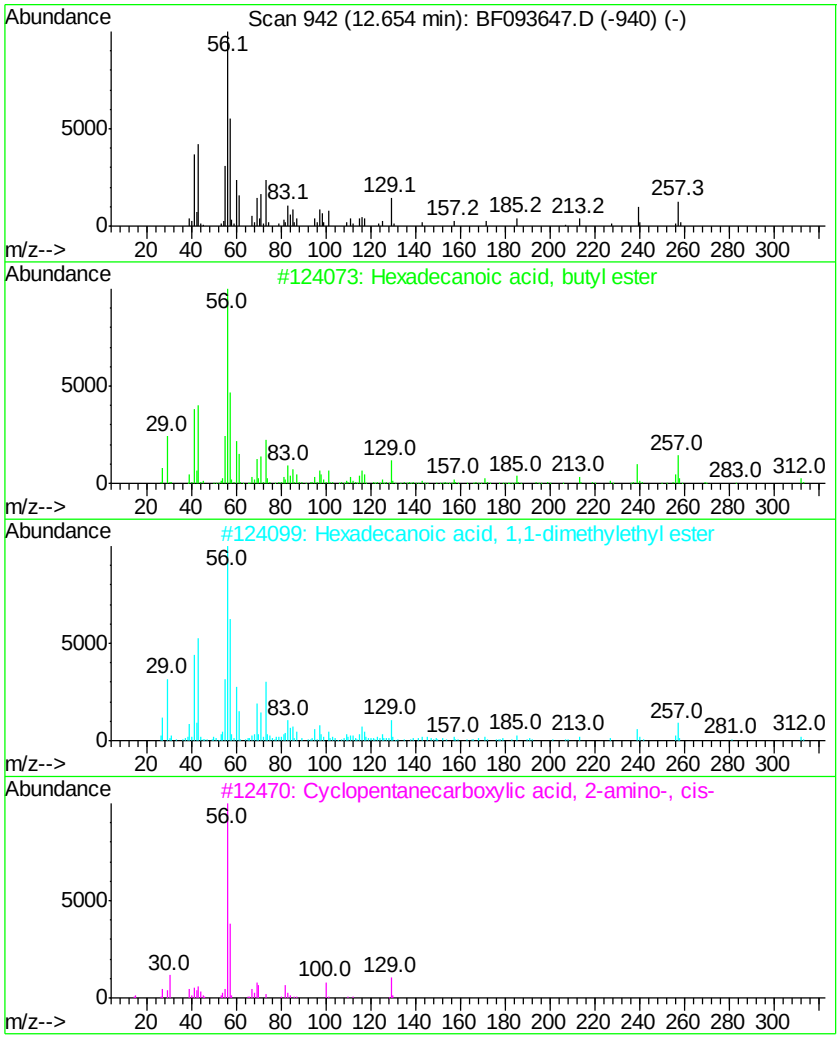
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

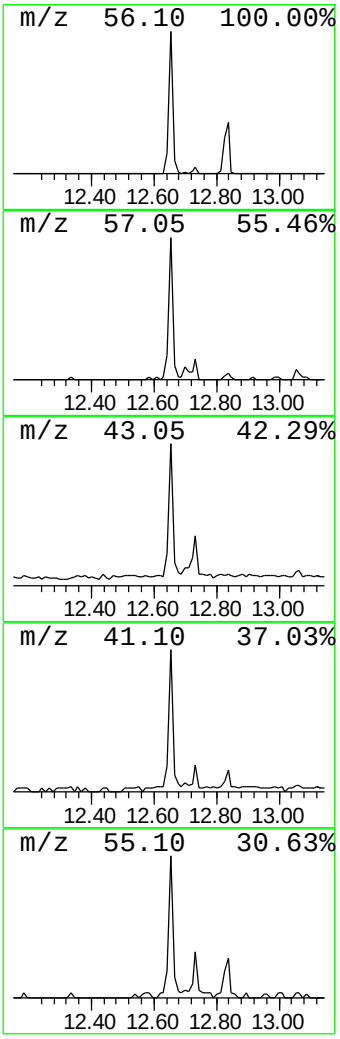
****

Peak Number 8 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	2.86 ng	157604	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	58
3	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43
4	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	43
5	2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	37





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
Data File : BF093647.D
Acq On : 14 Mar 2017 9:52
Operator : SJ/MA
Sample : I2201-23
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-126

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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
n-Propyl acetate	2.44	3.0	ng	152369	1	6.71	998486	20.0
4-Penten-2-one, 4...	3.14	2.8	ng	137108	1	6.71	998486	20.0
3-Hexen-2-one	4.17	21.0	ng	1047090	1	6.71	998486	20.0
2-Pentanone, 4-hy...	4.87	34.0	ng	1697390	1	6.71	998486	20.0
2-Pentanone, 4-me...	5.73	2.1	ng	106857	1	6.71	998486	20.0
unknown6.48	6.48	94.5	ng	4715230	1	6.71	998486	20.0
Hexadecanoic acid...	12.65	2.9	ng	157604	5	13.90	1100800	20.0