LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042915\
Data File : BF078842.D
Acq On : 30 Apr 2015 7:04
Operator : TP/IZ
Sample : G2021-13
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-25-5-10

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-BF042815.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	1.278	5	8	12	rVB	3096787	5696379	58.82%	11.503%
2	1.438	20	22	28	rVB	140766	245754	2.54%	0.496%
3	1.541	28	31	34	rVB	7921477	9684370	100.00%	19.555%
4	1.678	40	43	46	rVB	2390814	3925150	40.53%	7.926%
5	1.781	51	52	57	rBV	652933	922955	9.53%	1.864%
6	1.861	57	59	62	rVB	903659	1281380	13.23%	2.587%
7	1.918	62	64	88	rVB	2238265	3982731	41.13%	8.042%
8	2.216	88	90	105	rVB	52180	144871	1.50%	0.293%
9	5.153	345	347	349	rBV	100094	120820	1.25%	0.244%
10	5.187	349	350	360	rVB	260673	323625	3.34%	0.653%
11	5.679	390	393	396	rBV	2347333	2288730	23.63%	4.622%
12	6.925	500	502	505	rBV	2144051	2376447	24.54%	4.799%
13	7.096	514	517	519	rBV	1985690	2497522	25.79%	5.043%
14	7.382	540	542	544	rBV	501097	447410	4.62%	0.903%
15	7.565	556	558	561	rVB	1455142	1880914	19.42%	3.798%
16	8.068	600	602	605	rBV	1258639	1427475	14.74%	2.882%
17	8.959	678	680	683	rBV	736213	635006	6.56%	1.282%
18	10.308	795	798	800	rBV	3580473	3081323	31.82%	6.222%
19	11.142	868	871	873	rBV	610340	692482	7.15%	1.398%
20	12.114	954	956	959	rBV2	1553814	1852155	19.13%	3.740%
21	12.982	1030	1032	1034	rBV	723092	718444	7.42%	1.451%
22	14.983	1204	1207	1210	rBV	3319341	3492016	36.06%	7.051%
23	16.286	1318	1321	1323	rBV	844798	862520	8.91%	1.742%
24	18.057	1472	1476	1484	rVB	587227	942432	9.73%	1.903%

Sum of corrected areas: 49522911

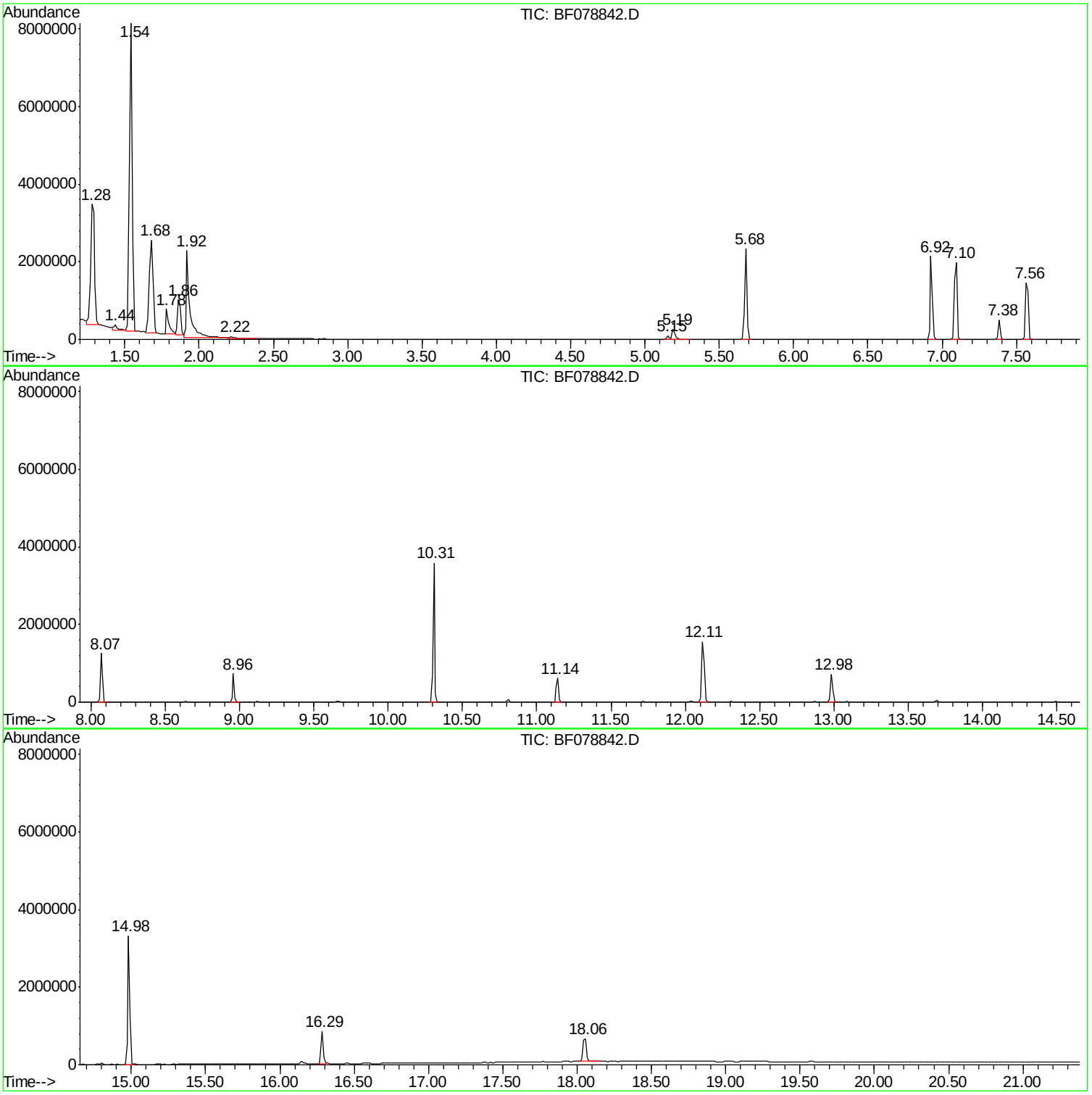
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042915\
Data File : BF078842.D
Acq On : 30 Apr 2015 7:04
Operator : TP/IZ
Sample : G2021-13
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-25-5-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.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 F\DATA\BF042915\
Data File : BF078842.D
Acq On : 30 Apr 2015 7:04
Operator : TP/IZ
Sample : G2021-13
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-25-5-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

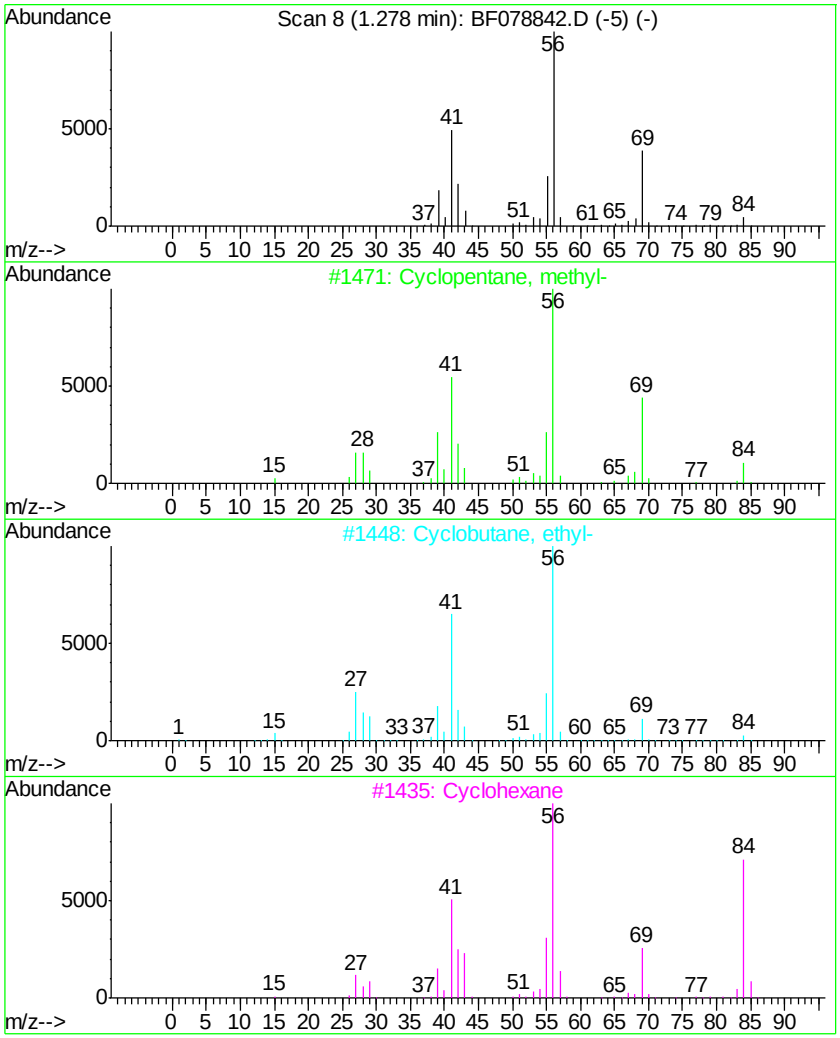
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

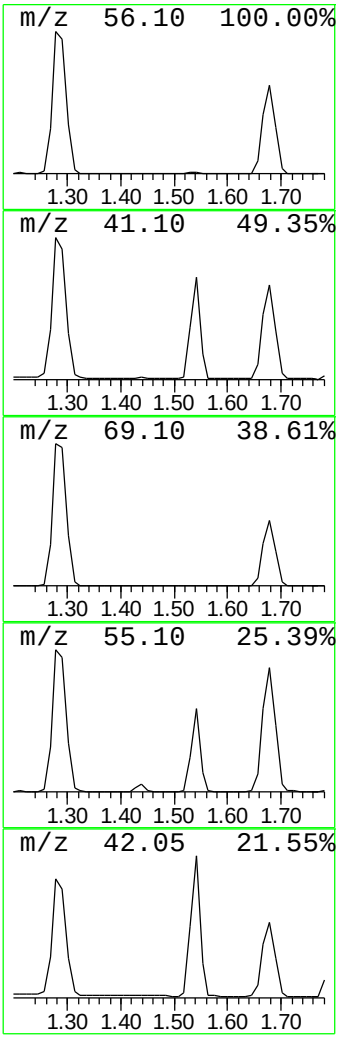
****

Peak Number 1 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.28	254.64 ng	5696380	1,4-Dichlorobenzene-d4	7.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	87
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	86
3	Cyclohexane	84	C6H12	000110-82-7	78
4	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	72
5	2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	45





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042915\
Data File : BF078842.D
Acq On : 30 Apr 2015 7:04
Operator : TP/IZ
Sample : G2021-13
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-25-5-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.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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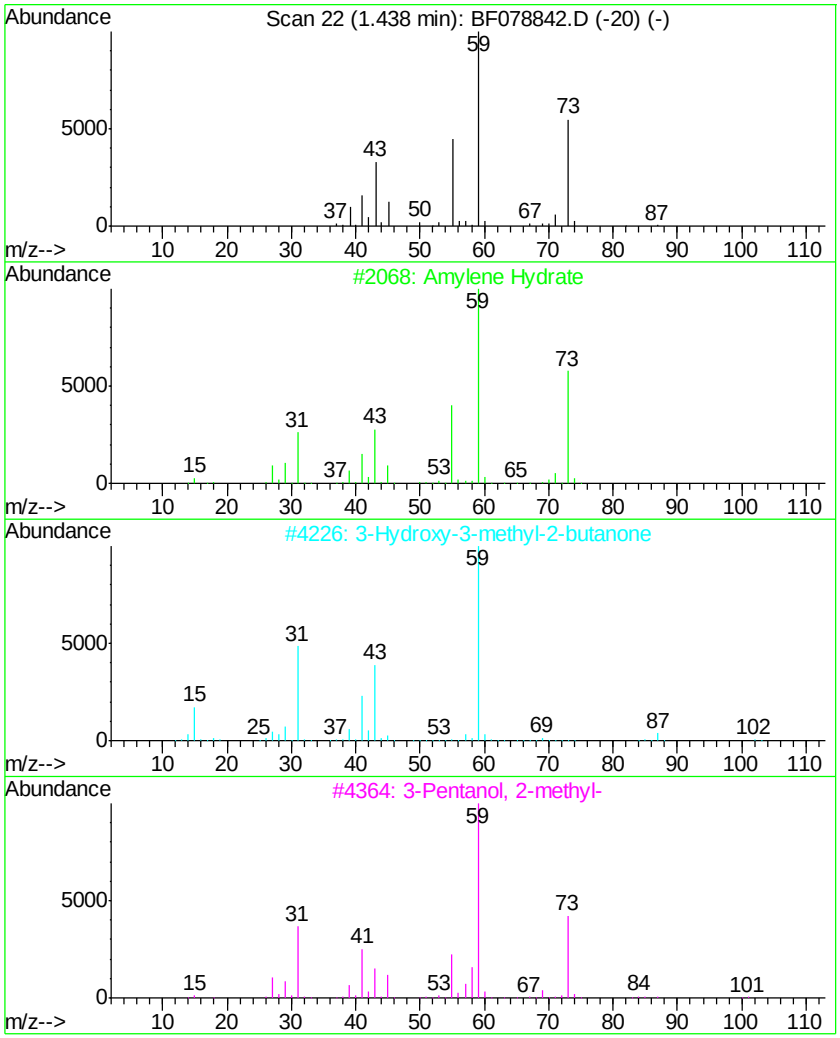
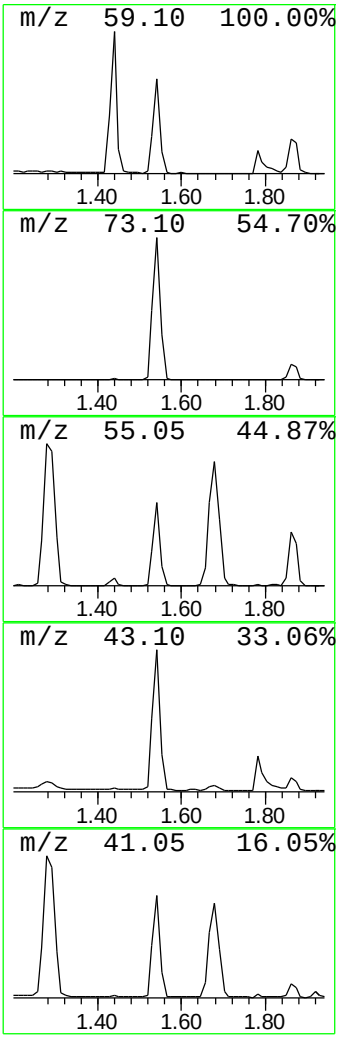
Peak Number 2 Amylene Hydrate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.44	10.99 ng	245754	1,4-Dichlorobenzene-d4	7.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Amylene Hydrate	88	C5H12O	000075-85-4	83
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	42
3	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	39
4	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	36
5	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042915\
Data File : BF078842.D
Acq On : 30 Apr 2015 7:04
Operator : TP/IZ
Sample : G2021-13
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-25-5-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

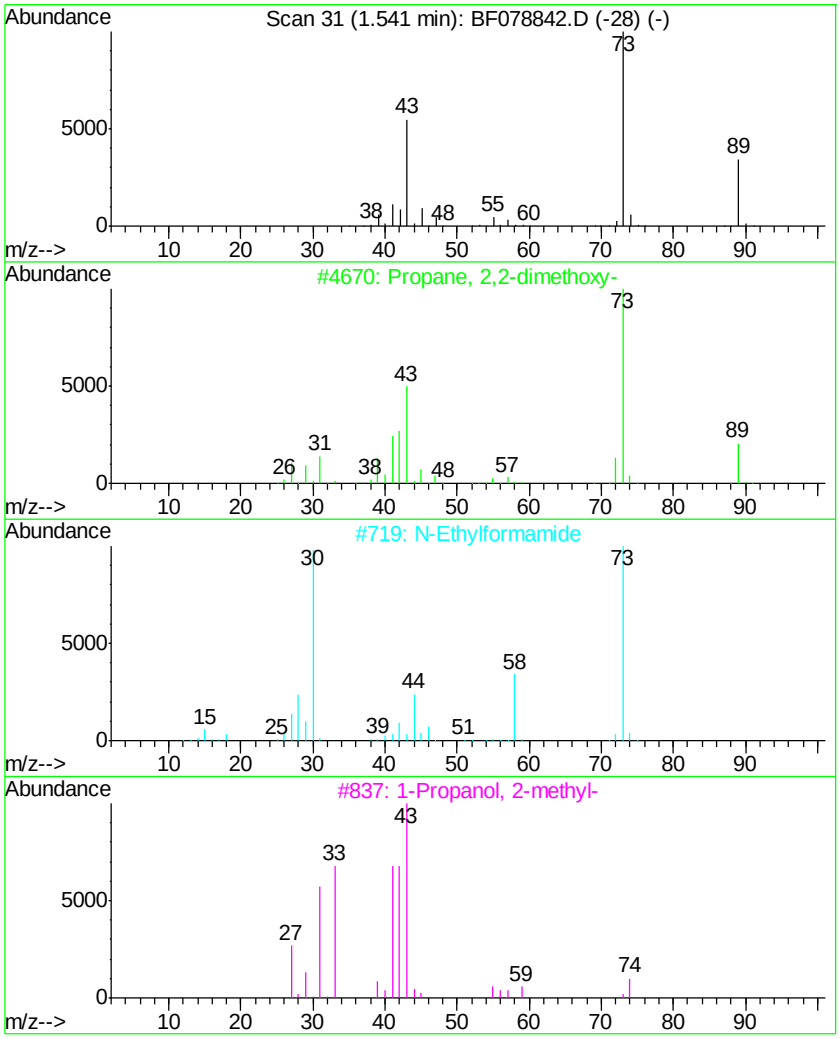
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

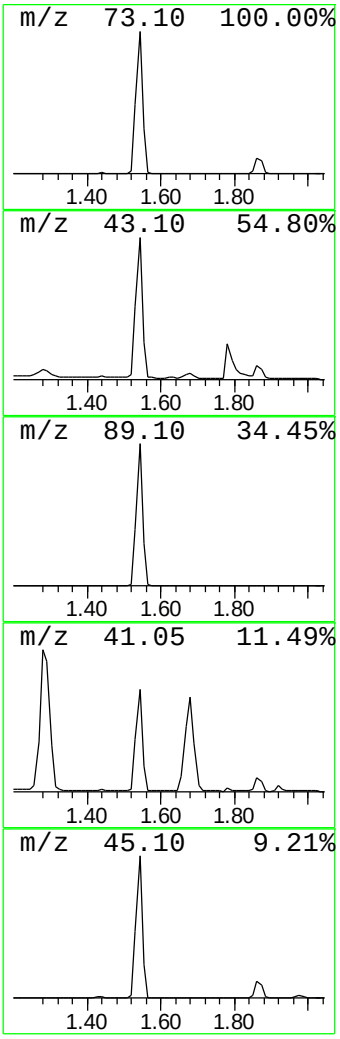
****

Peak Number 3 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.54	432.91 ng	9684370	1,4-Dichlorobenzene-d4	7.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
4	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042915\
Data File : BF078842.D
Acq On : 30 Apr 2015 7:04
Operator : TP/IZ
Sample : G2021-13
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-25-5-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

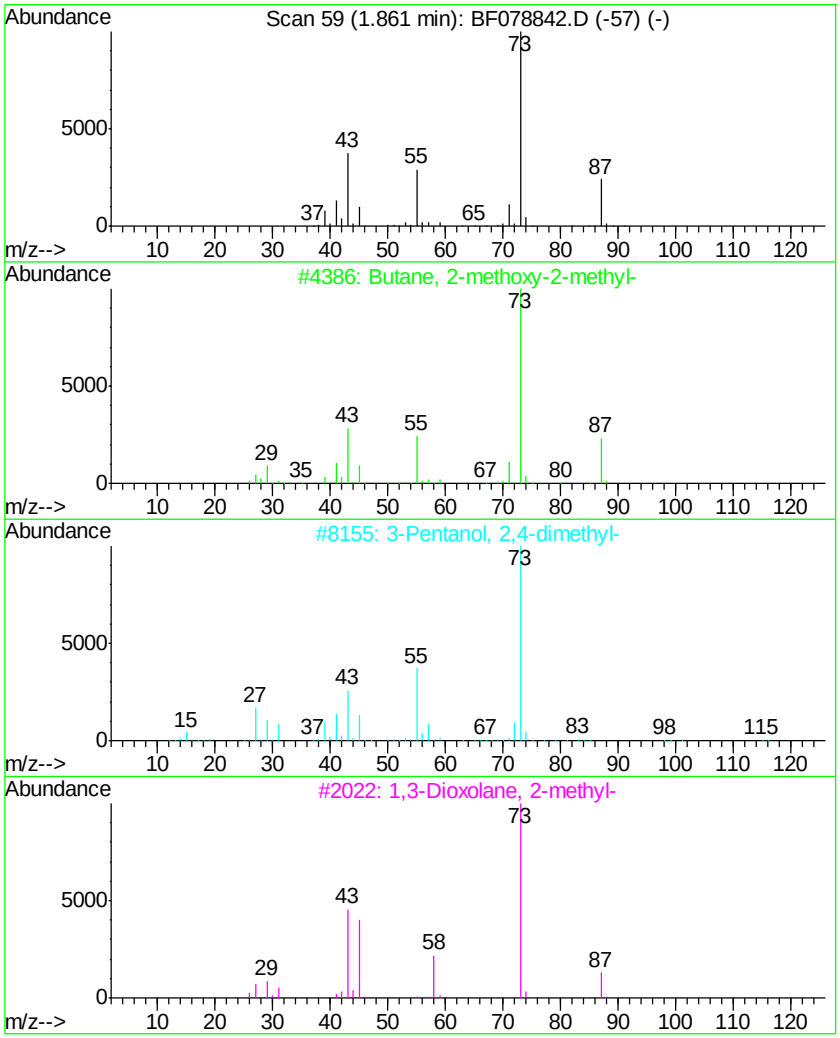
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

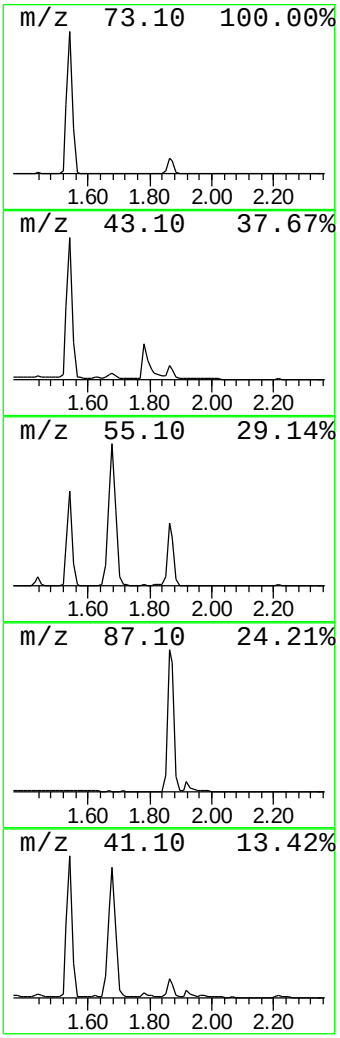
****

Peak Number 6 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.86	57.28 ng	1281380	1,4-Dichlorobenzene-d4	7.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042915\
Data File : BF078842.D
Acq On : 30 Apr 2015 7:04
Operator : TP/IZ
Sample : G2021-13
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-25-5-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

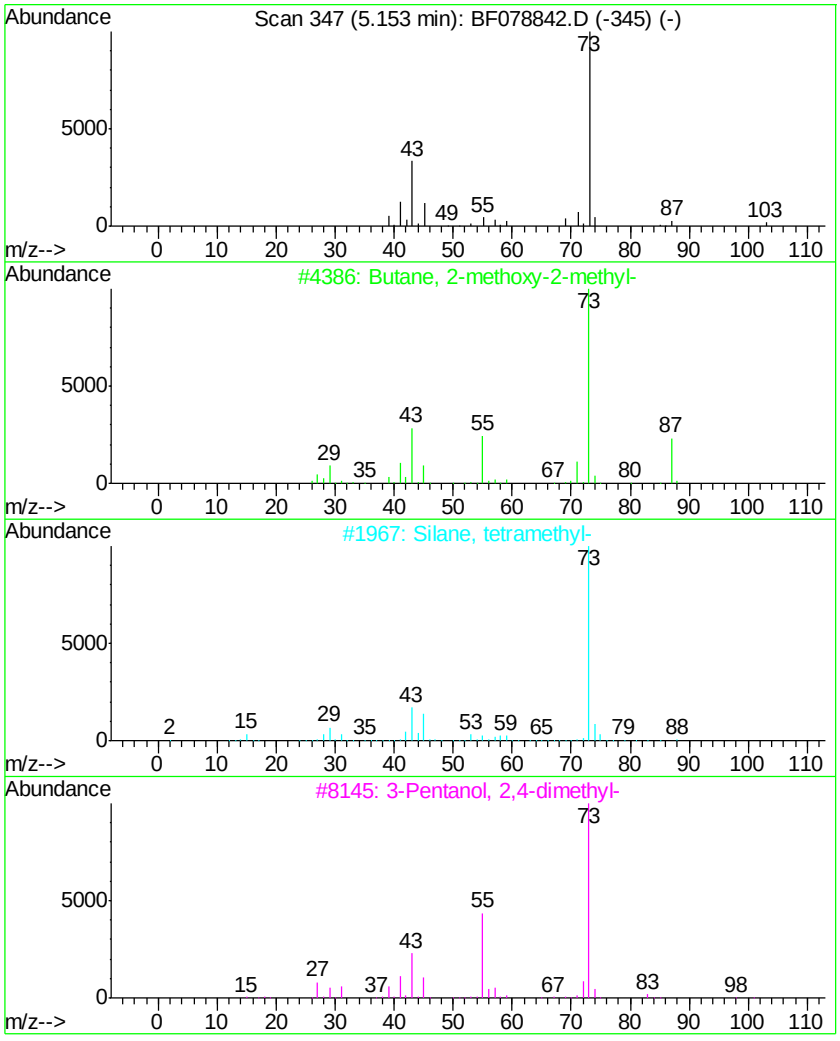
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

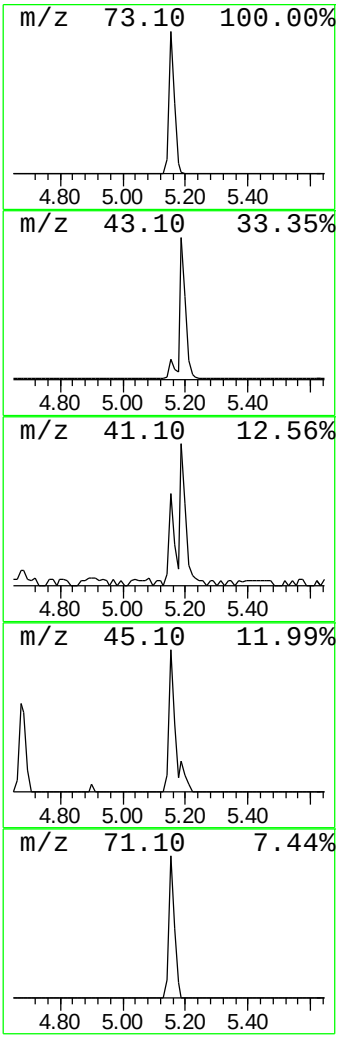
****

Peak Number 9 unknown5.15 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	5.40 ng	120820	1,4-Dichlorobenzene-d4	7.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	33
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	33
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9
4	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
5	Acetic acid, 3-[1,3]dioxolan-2-y...	174	C8H14O4	1000186-02-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042915\
Data File : BF078842.D
Acq On : 30 Apr 2015 7:04
Operator : TP/IZ
Sample : G2021-13
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-25-5-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

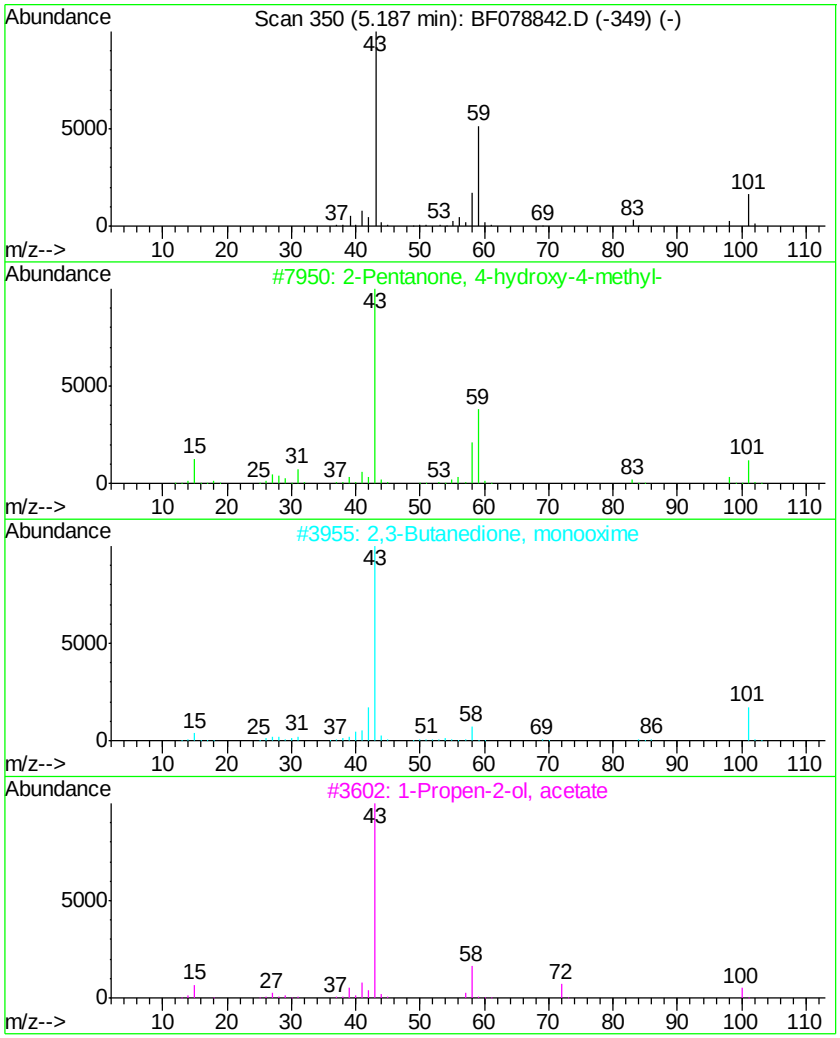
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

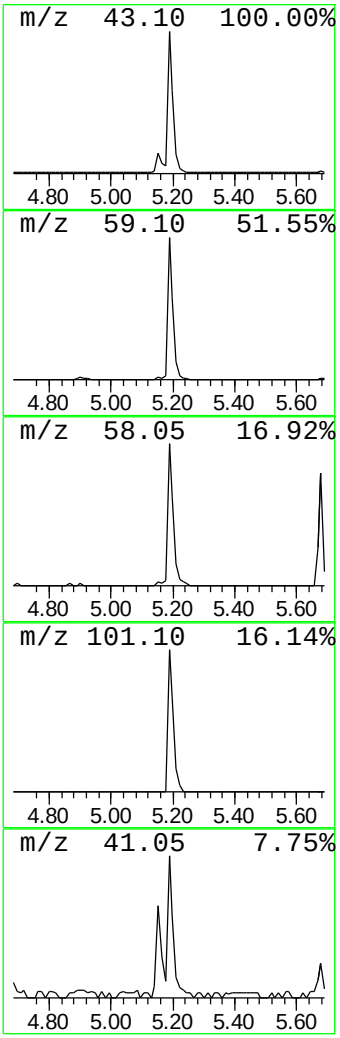
****

Peak Number 10 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	14.47 ng	323625	1,4-Dichlorobenzene-d4	7.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9





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Data File : BF078842.D
Acq On : 30 Apr 2015 7:04
Operator : TP/IZ
Sample : G2021-13
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-25-5-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

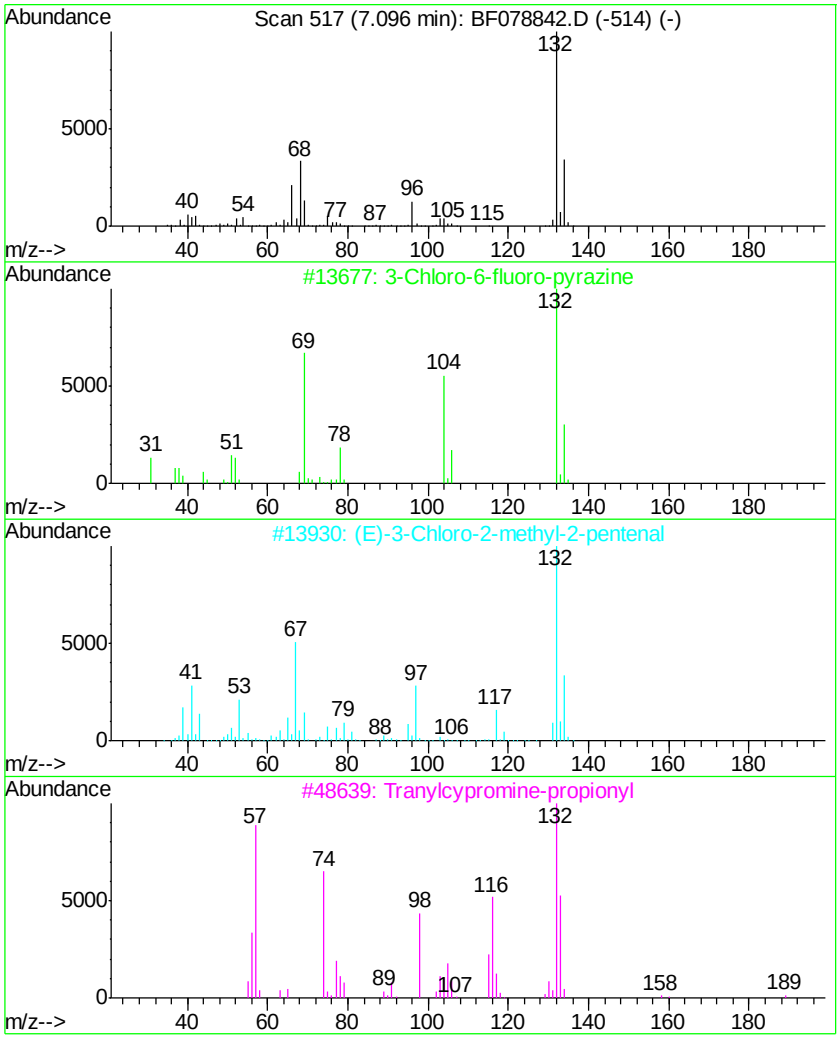
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

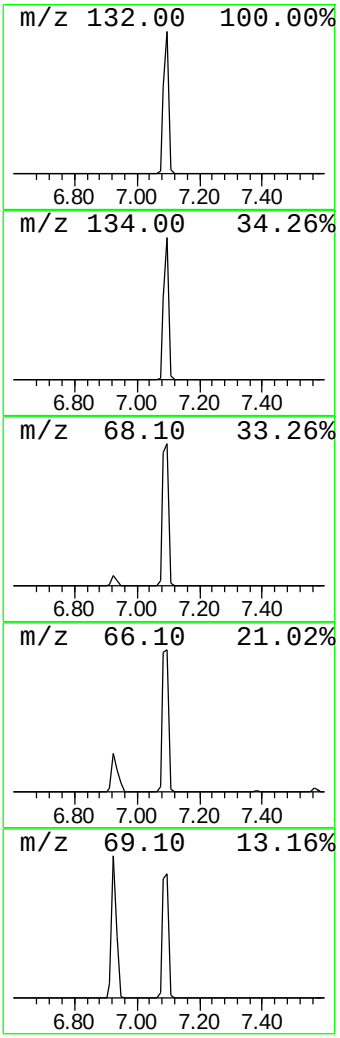
****

Peak Number 11 unknown7.10 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.10	111.64 ng	2497520	1,4-Dichlorobenzene-d4	7.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Amphetaminil	250	C17H18N2	017590-01-1	12
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042915\
Data File : BF078842.D
Acq On : 30 Apr 2015 7:04
Operator : TP/IZ
Sample : G2021-13
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-25-5-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.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
Cyclopentane, met...	1.28	254.6	ng	5696380	1	7.38	447410	20.0
Amylene Hydrate	1.44	11.0	ng	245754	1	7.38	447410	20.0
Propane, 2,2-dime...	1.54	432.9	ng	9684370	1	7.38	447410	20.0
Butane, 2-methoxy...	1.86	57.3	ng	1281380	1	7.38	447410	20.0
unknown5.15	5.15	5.4	ng	120820	1	7.38	447410	20.0
2-Pentanone, 4-hy...	5.19	14.5	ng	323625	1	7.38	447410	20.0
unknown7.10	7.10	111.6	ng	2497520	1	7.38	447410	20.0