

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016613.D
 Acq On : 30 Sep 2021 23:22
 Operator : CG/JU
 Sample : M3833-09
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 RE103D2-20210920

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : OFF Filtering: 5
 Sampling : 1 Min Area: 1 % 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:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BN016613.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.198	5	13	30	rVB	1645952	4606544	100.00%	65.981%
2	4.821	186	189	204	rVB	414191	764355	16.59%	10.948%
3	7.642	491	495	500	rBV	53245	94616	2.05%	1.355%
4	8.784	602	605	610	rBV	27215	49443	1.07%	0.708%
5	10.191	713	716	721	rBV	45360	75651	1.64%	1.084%
6	10.407	730	733	736	rBV	97388	167792	3.64%	2.403%
7	12.003	921	931	943	rBV	48557	79978	1.74%	1.146%
8	12.898	1071	1075	1078	rBV	94732	175450	3.81%	2.513%
9	14.269	1180	1183	1190	rBV	123702	186178	4.04%	2.667%
10	17.017	1400	1403	1406	rBV	89866	146041	3.17%	2.092%
11	19.063	1688	1696	1722	rBV	117510	162914	3.54%	2.333%
12	19.678	1813	1820	1855	rBV	108141	142925	3.10%	2.047%
13	21.227	1998	2001	2011	rVV	116424	166020	3.60%	2.378%
14	23.481	2413	2426	2467	rVB	80563	163715	3.55%	2.345%

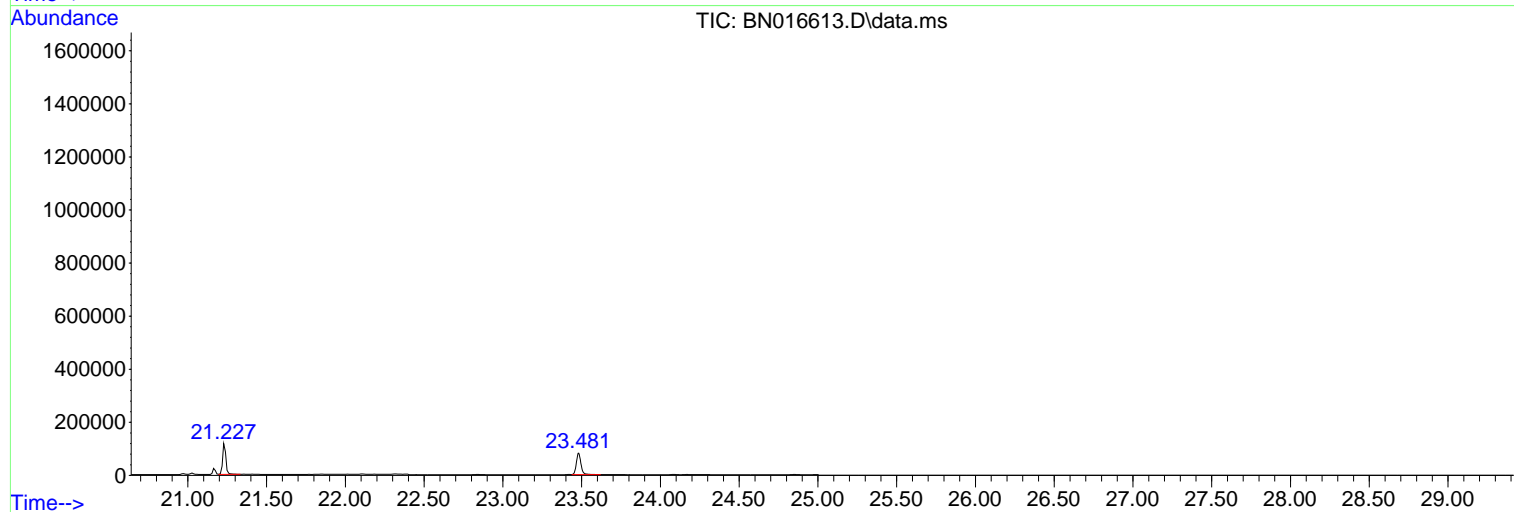
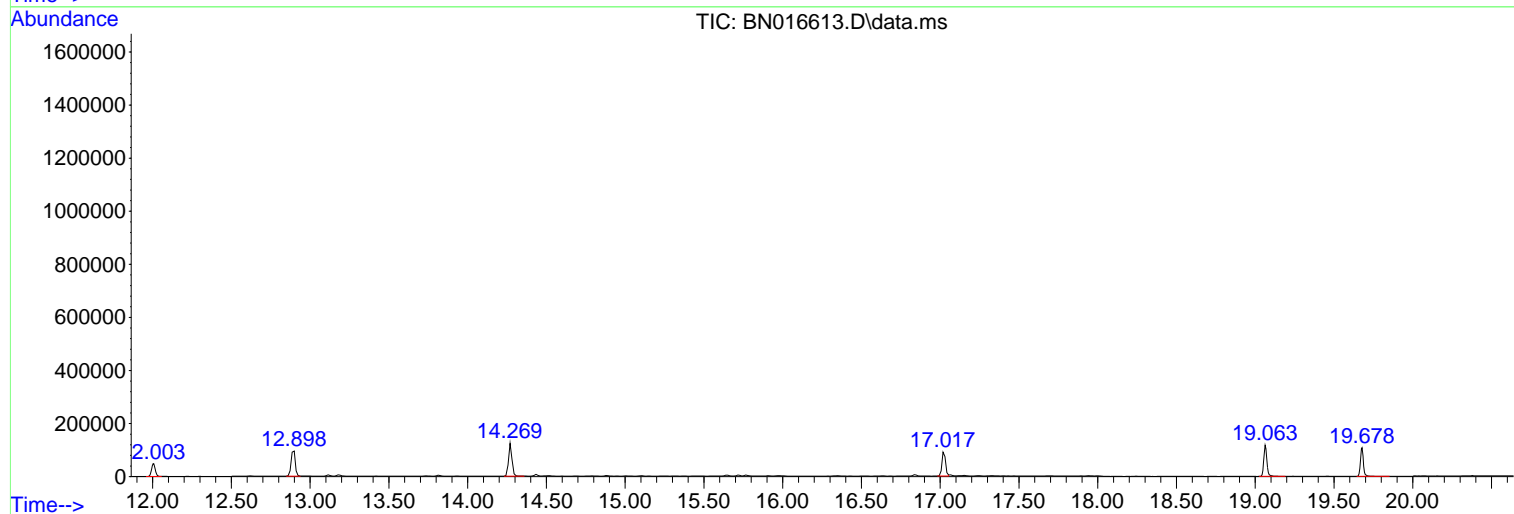
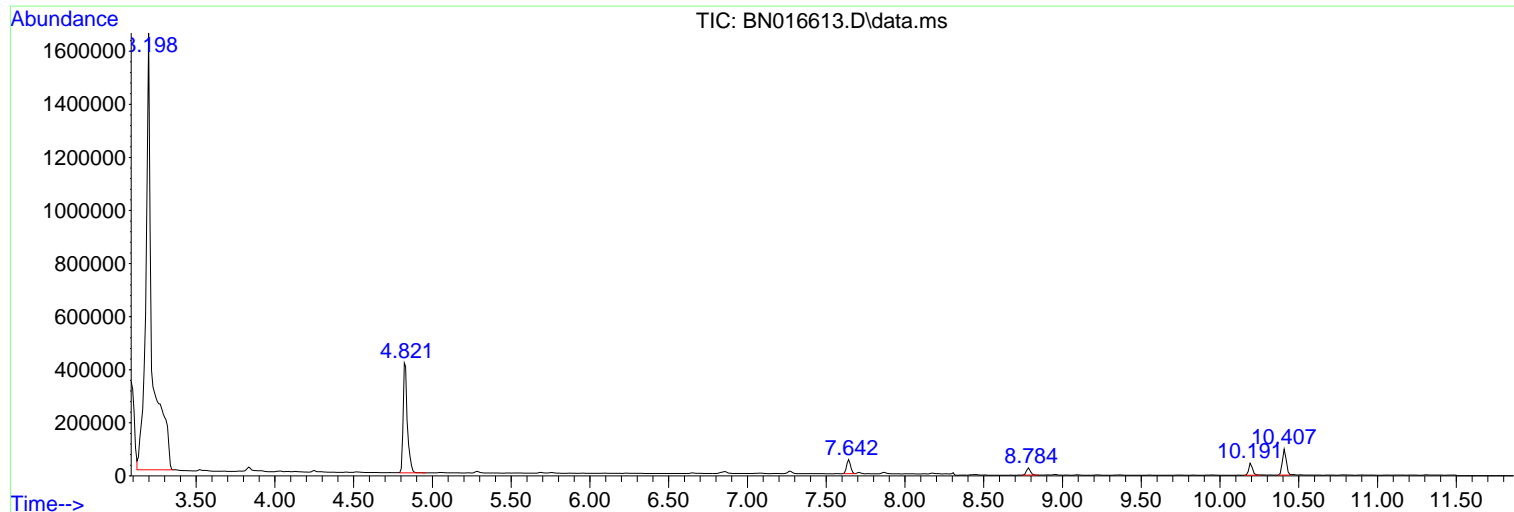
Sum of corrected areas: 6981622

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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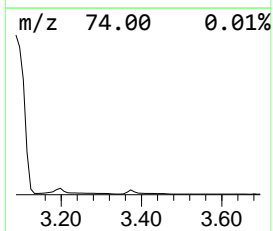
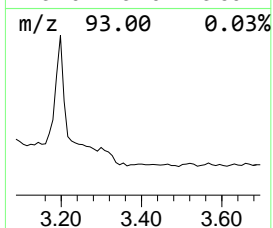
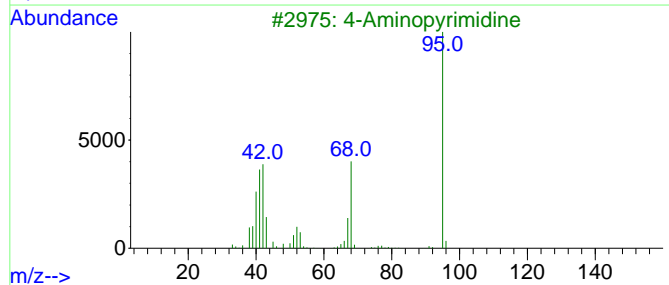
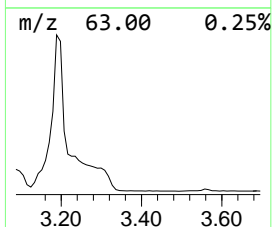
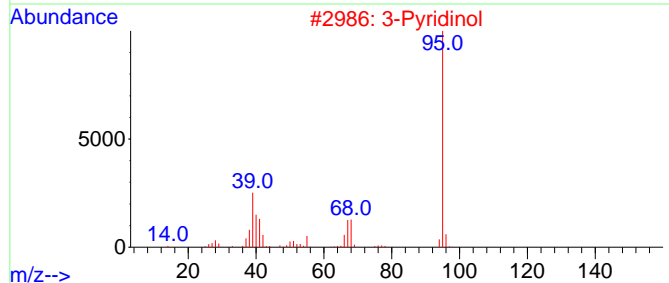
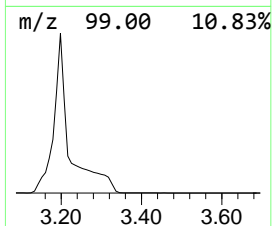
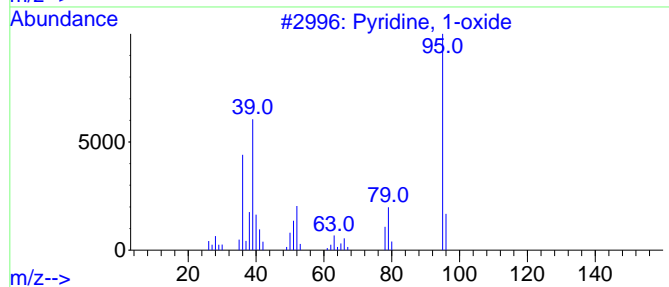
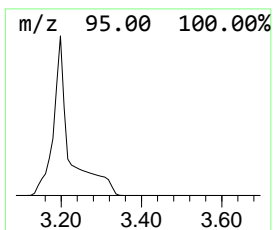
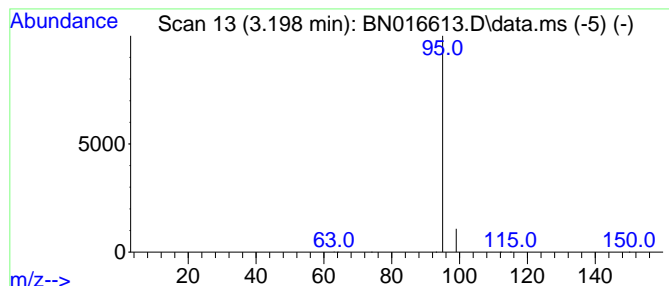
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 1 Pyridine, 1-oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.198	19.47 ng	4606540	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyridine, 1-oxide	95	C5H5NO	000694-59-7	2
2			3-Pyridinol	95	C5H5NO	000109-00-2	2
3			4-Aminopyrimidine	95	C4H5N3	000591-54-8	2
4			4-Pyridinol	95	C5H5NO	000626-64-2	2
5			2-(Aminomethylene)aminoacrylontrile	95	C4H5N3	167320-31-2	2



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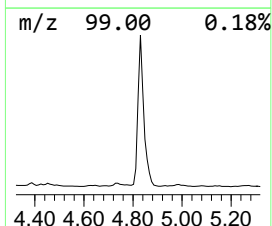
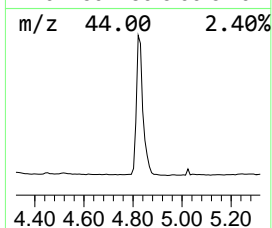
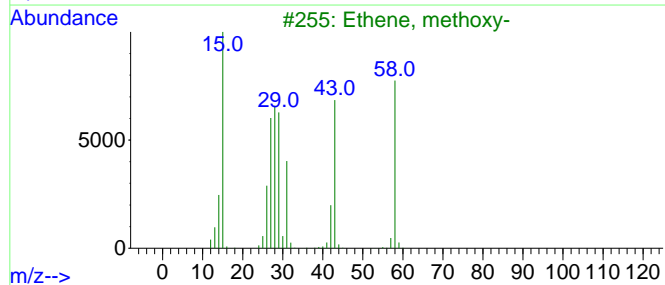
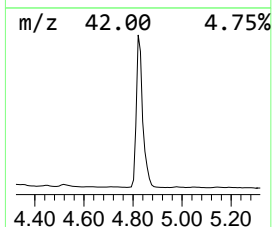
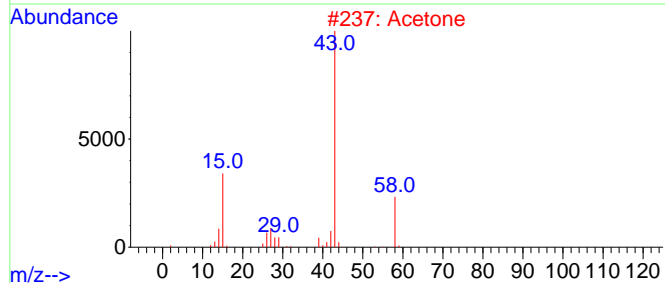
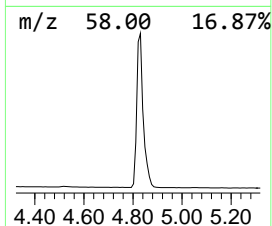
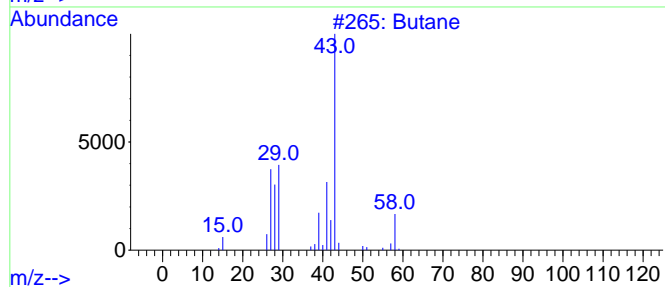
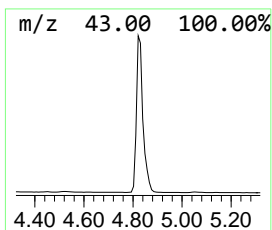
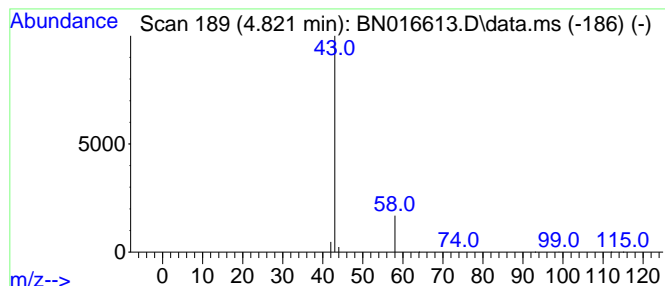
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 Peak Number 2 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	3.23 ng	764355	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	4
2			Acetone	58	C3H6O	000067-64-1	4
3			Ethene, methoxy-	58	C3H6O	000107-25-5	3
4			Diazene, dimethyl-	58	C2H6N2	000503-28-6	3
5			Hydrogen isocyanate	43	CHNO	000075-13-8	2



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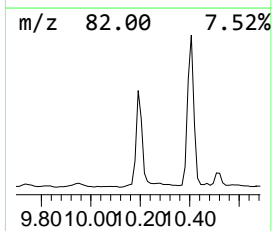
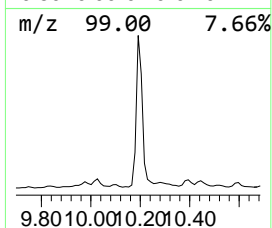
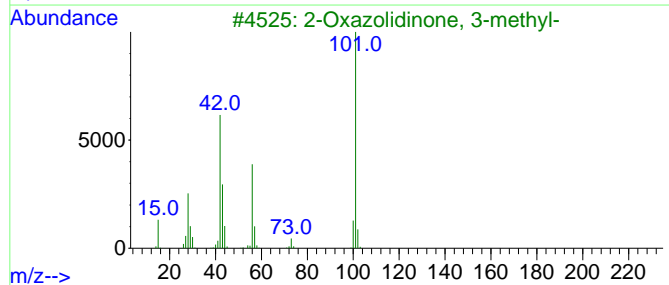
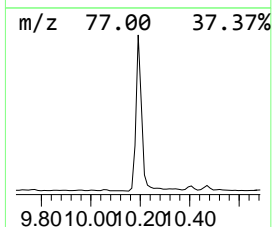
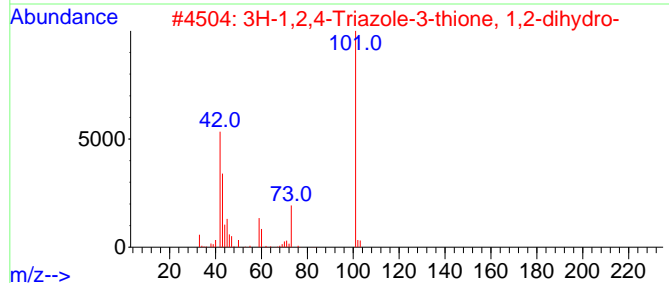
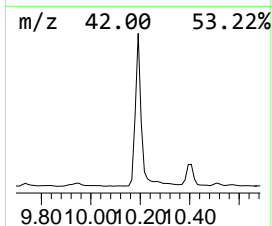
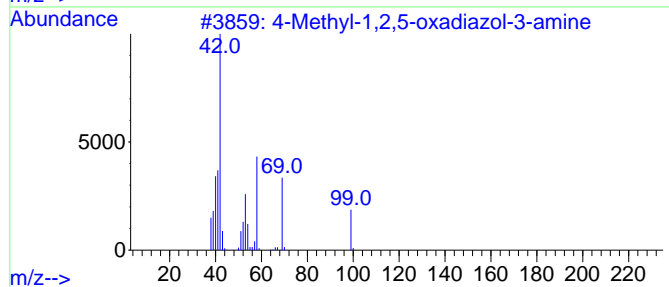
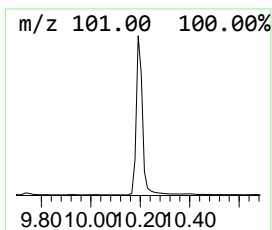
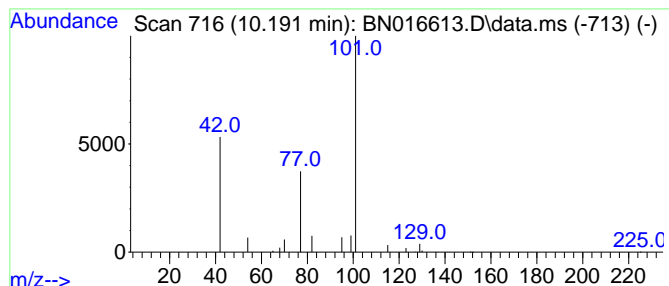
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 Peak Number 3 4-Methyl-1,2,5-oxadiazol-3-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.18 ng	75651	Naphthalene-d8	10.406

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Methyl-1,2,5-oxadiazol-3-amine	99	C3H5N3O	1000411-31-0	5
2		3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
3		2-Oxazolidinone, 3-methyl-	101	C4H7N2O2	019836-78-3	5
4		Morpholine, 2,5,5-trimethyl-	129	C7H15NO	1000460-73-8	5
5		Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	5



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pyridine, 1-oxide	3.198	19.5	ng	4606540	1	7.642	94616	0.4
Butane	4.821	3.2	ng	764355	1	7.642	94616	0.4
4-Methyl-1,2,5-...	10.191	0.2	ng	75651	2	10.406	167792	0.4