

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100923\
 Data File : BF135661.D
 Acq On : 09 Oct 2023 20:40
 Operator : CG\JU
 Sample : 04656-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-105D

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:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135661.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.775	282	287	295	rBV2	21648	39165	1.11%	0.209%
2	4.963	485	489	498	rBV2	32849	56516	1.61%	0.301%
3	5.375	555	559	576	rBV	1306433	1568531	44.55%	8.363%
4	6.387	729	731	748	rBV	729368	822939	23.37%	4.388%
5	6.740	787	791	800	rBV	803420	707316	20.09%	3.771%
6	7.310	883	888	896	rBV	2251186	2208059	62.71%	11.773%
7	8.016	1005	1008	1020	rBV	1062695	925385	26.28%	4.934%
8	9.098	1187	1192	1195	rBV	3953570	3520978	100.00%	18.774%
9	9.216	1208	1212	1222	rVB	469102	473341	13.44%	2.524%
10	9.775	1303	1307	1314	rVB	1140287	950995	27.01%	5.071%
11	10.575	1438	1443	1458	rBV	2047575	2141353	60.82%	11.418%
12	11.269	1558	1561	1571	rBV	1118232	940670	26.72%	5.016%
13	11.804	1649	1652	1664	rBV2	97488	134480	3.82%	0.717%
14	12.374	1747	1749	1756	rVB2	134885	117652	3.34%	0.627%
15	12.598	1783	1787	1792	rBV3	22397	38278	1.09%	0.204%
16	12.869	1828	1833	1836	rBV	2878488	2696451	76.58%	14.377%
17	13.933	2010	2014	2021	rVB	715667	665822	18.91%	3.550%
18	14.774	2154	2157	2161	rVB2	47293	54245	1.54%	0.289%
19	15.404	2259	2264	2273	rBV	498105	692741	19.67%	3.694%

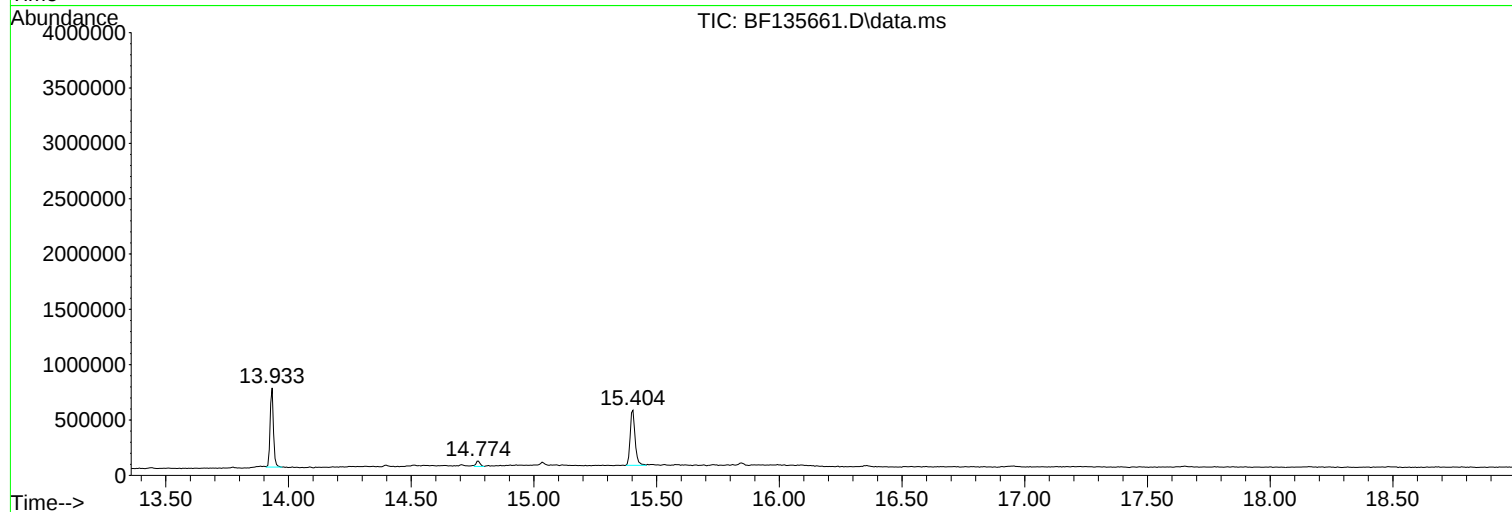
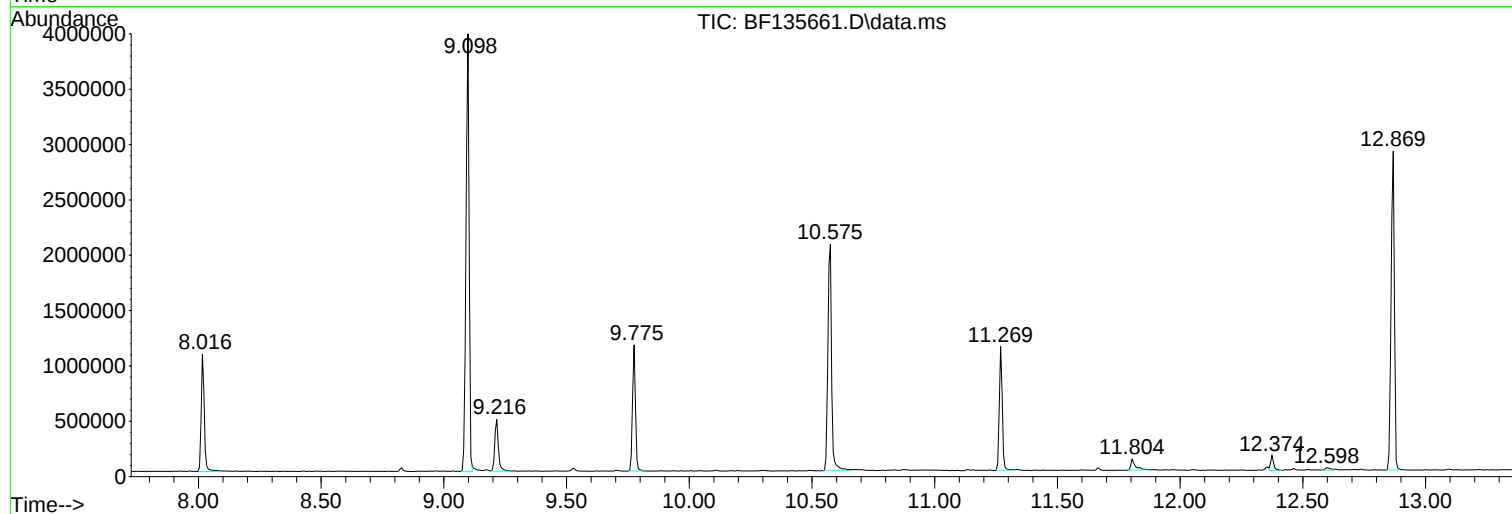
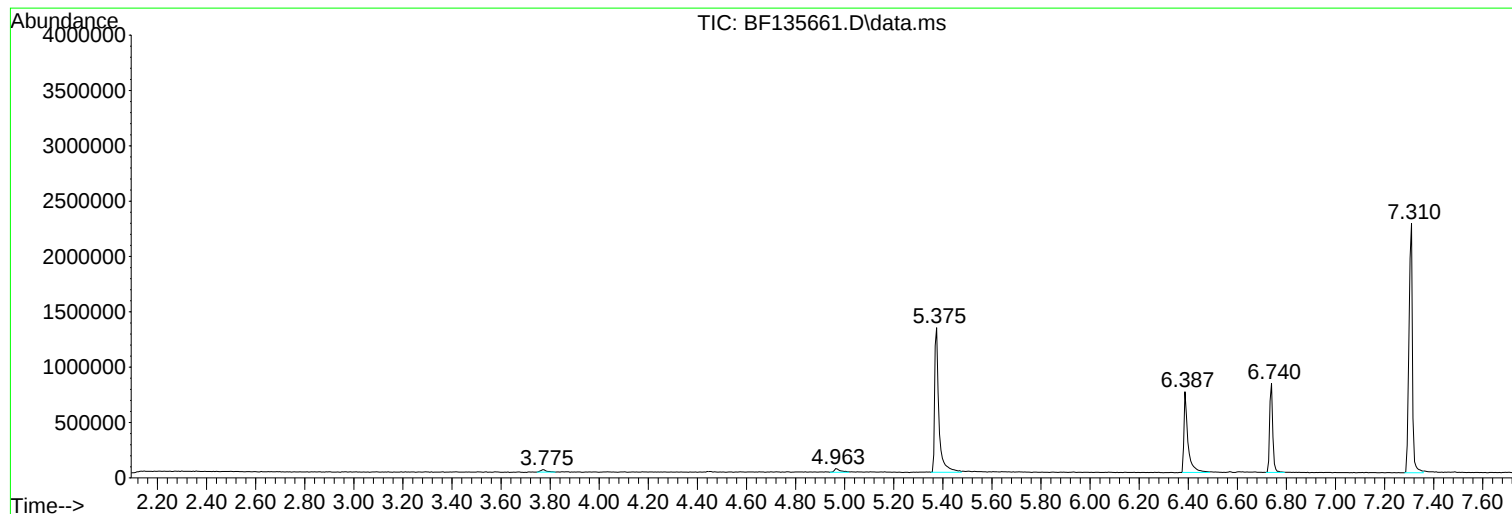
Sum of corrected areas: 18754917

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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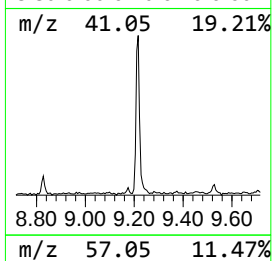
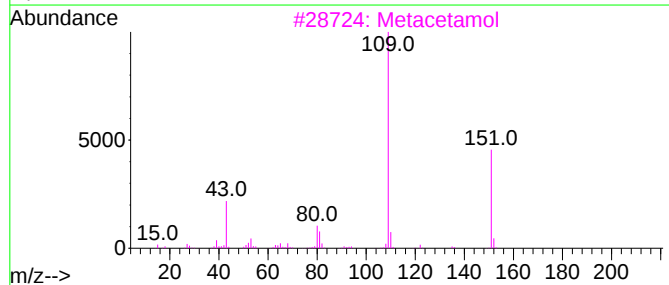
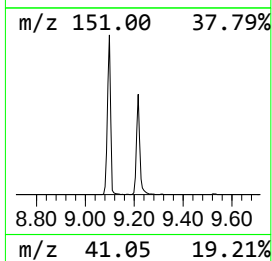
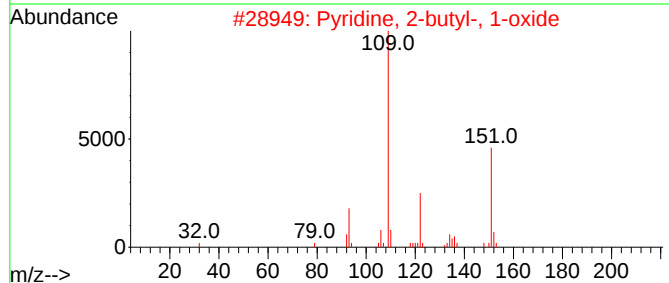
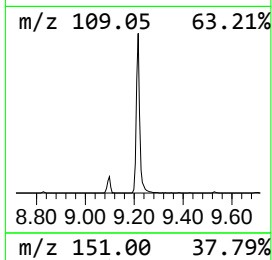
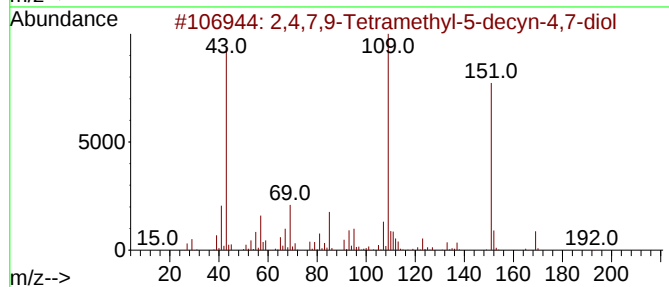
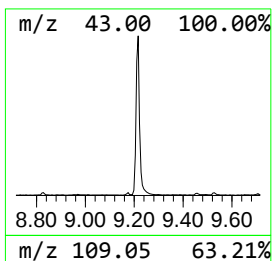
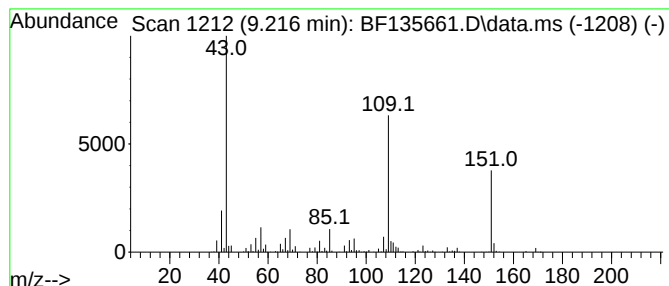
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Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.216	9.95 ng	473341	Acenaphthene-d10	9.775

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	87	
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53	
3	Metacetamol	151	C8H9NO2	000621-42-1	49	
4	Acetaminophen	151	C8H9NO2	000103-90-2	47	
5	2-Thiophenecarbonitrile	109	C5H3NS	001003-31-2	43	



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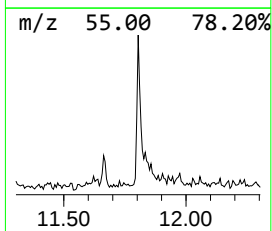
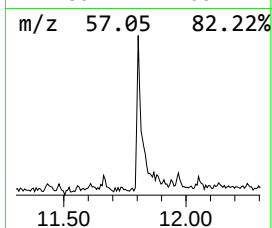
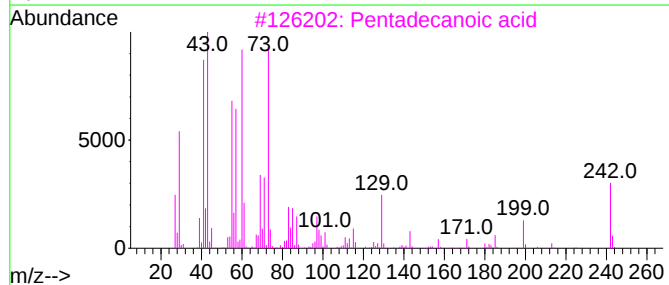
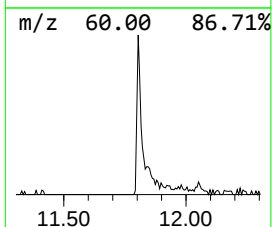
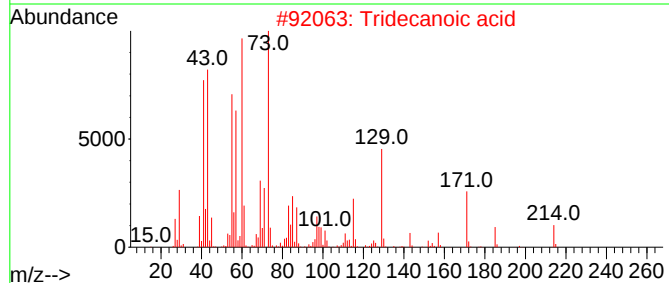
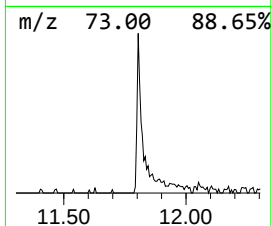
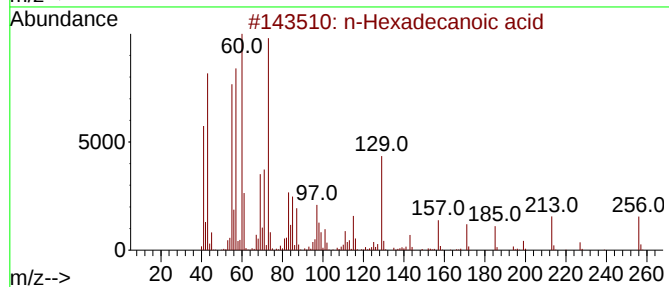
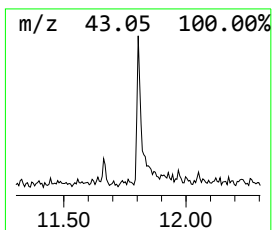
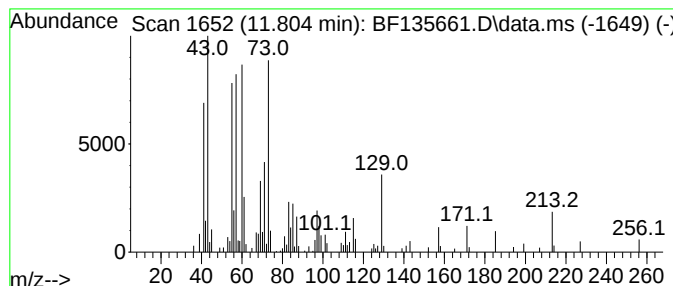
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	2.86 ng	134480	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2			Tridecanoic acid	214	C13H26O2	000638-53-9	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4			n-Decanoic acid	172	C10H20O2	000334-48-5	62
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	53



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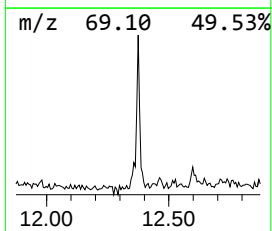
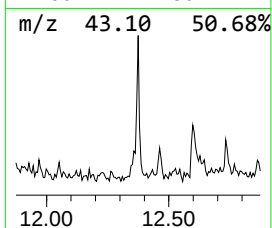
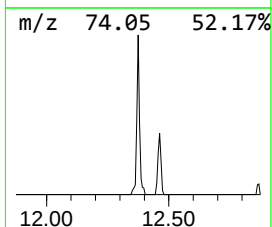
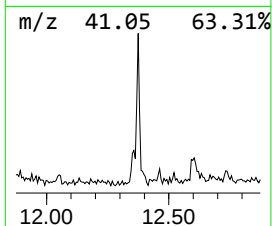
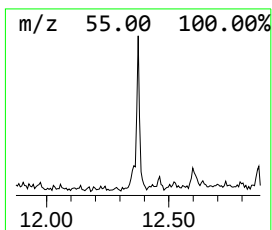
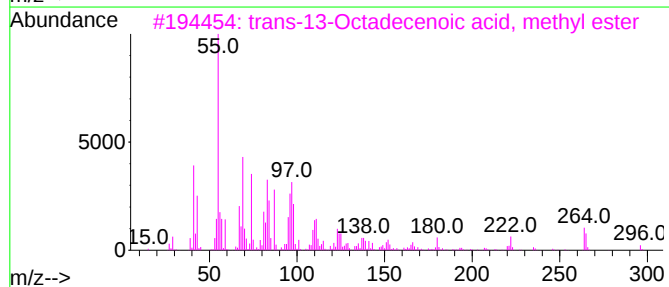
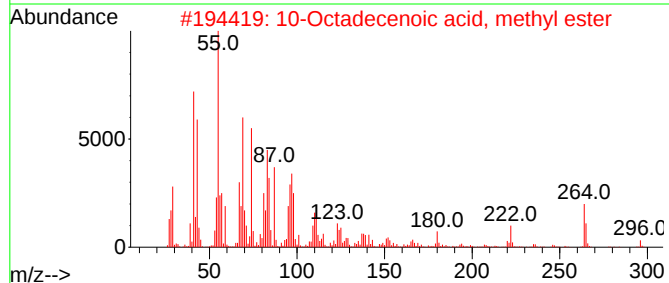
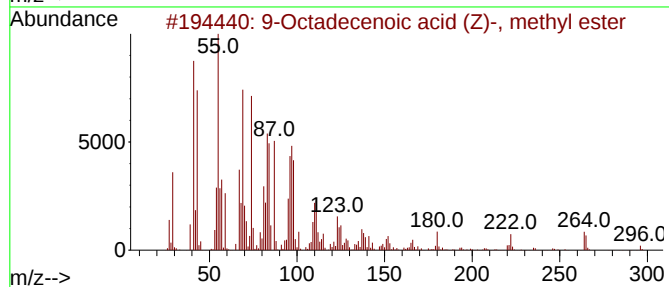
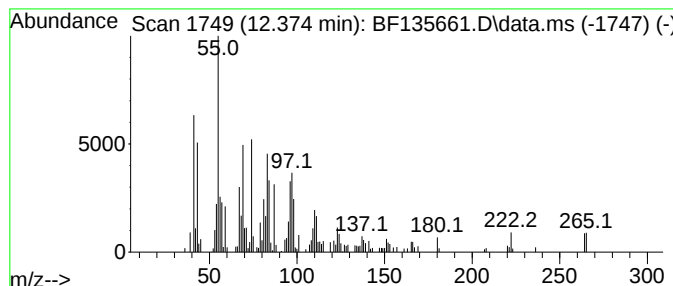
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Peak Number 3 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.374	2.50 ng	117652	Phenanthrene-d10	11.269	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	94
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
3	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	91
4	6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	87
5	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2,4,7,9-Tetrame...	9.216	9.9	ng	473341	3	9.775	950995	20.0
n-Hexadecanoic ...	11.804	2.9	ng	134480	4	11.269	940670	20.0
9-Octadecenoic ...	12.374	2.5	ng	117652	4	11.269	940670	20.0