

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051622\
 Data File : VU048589.D
 Acq On : 16 May 2022 18:47
 Operator : SY/MD
 Sample : N2849-01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXXW6

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % 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:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
 Title : VOC Analysis

Signal : TIC: VU048589.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	73	81	98	rVB	93285	103851	11.18%	1.287%
2	1.913	170	178	193	rVB	72615	93952	10.12%	1.164%
3	2.205	263	269	274	rBV4	1194	1591	0.17%	0.020%
4	2.273	284	290	297	rBV4	1194	1483	0.16%	0.018%
5	2.568	366	382	394	rBV	193021	323274	34.81%	4.005%
6	2.755	431	440	451	rBV2	2627	4945	0.53%	0.061%
7	2.903	482	486	491	rVB2	575	522	0.06%	0.006%
8	2.938	492	497	500	rBV	331	328	0.04%	0.004%
9	2.957	500	503	506	rBV	410	328	0.04%	0.004%
10	3.051	526	532	534	rBV2	636	490	0.05%	0.006%
11	3.183	559	573	585	rBV3	3581	8435	0.91%	0.105%
12	3.356	622	627	630	rBB	253	214	0.02%	0.003%
13	3.375	630	633	636	rBB2	303	228	0.02%	0.003%
14	3.411	640	644	646	rBV	177	183	0.02%	0.002%
15	3.527	677	680	683	rBB	291	168	0.02%	0.002%
16	3.646	713	717	720	rBV	190	212	0.02%	0.003%
17	3.855	776	782	787	rBB	267	290	0.03%	0.004%
18	4.006	825	829	832	rBB	309	261	0.03%	0.003%
19	4.189	881	886	890	rBV	286	294	0.03%	0.004%
20	4.269	908	911	913	rBV2	348	283	0.03%	0.004%
21	4.298	917	920	923	rVB2	302	191	0.02%	0.002%
22	4.449	959	967	969	rBV4	3712	4501	0.48%	0.056%
23	4.620	1008	1020	1043	rBV	96195	224479	24.17%	2.781%
24	4.832	1082	1086	1088	rBV	411	352	0.04%	0.004%
25	4.977	1127	1131	1132	rBV	371	273	0.03%	0.003%
26	5.067	1142	1159	1183	rBV	182222	429123	46.20%	5.316%
27	5.269	1218	1222	1225	rBV2	272	269	0.03%	0.003%
28	5.285	1225	1227	1229	rBV2	306	168	0.02%	0.002%
29	5.340	1241	1244	1247	rBV2	295	240	0.03%	0.003%
30	5.411	1263	1266	1268	rBB	312	170	0.02%	0.002%
31	5.462	1279	1282	1288	rVB2	370	270	0.03%	0.003%
32	5.726	1342	1364	1393	rBV2	332739	928775	100.00%	11.507%
33	5.864	1402	1407	1409	rBV2	428	447	0.05%	0.006%
34	5.938	1427	1430	1432	rBV	327	185	0.02%	0.002%
35	5.957	1432	1436	1443	rVV2	475	572	0.06%	0.007%
36	5.996	1444	1448	1450	rVV	393	293	0.03%	0.004%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051622\
 Data File : VU048589.D
 Acq On : 16 May 2022 18:47
 Operator : SY/MD
 Sample : N2849-01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXXW6

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % 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:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
 Title : VOC Analysis

37	6.044	1462	1463	1468	rVB2	360	256	0.03%	0.003%
38	6.131	1485	1490	1492	rBV	350	320	0.03%	0.004%
39	6.170	1500	1502	1505	rBB	358	207	0.02%	0.003%
40	6.195	1506	1510	1511	rBV	304	188	0.02%	0.002%
41	6.250	1514	1527	1550	rVV	298103	563748	60.70%	6.984%
42	6.498	1600	1604	1607	rBV2	419	392	0.04%	0.005%
43	6.530	1607	1614	1619	rBV5	2053	2989	0.32%	0.037%
44	6.690	1650	1664	1683	rBV	209641	404811	43.59%	5.015%
45	6.877	1712	1722	1738	rVV3	16728	32072	3.45%	0.397%
46	7.038	1766	1772	1774	rBV2	545	473	0.05%	0.006%
47	7.108	1781	1794	1805	rVB	15203	26872	2.89%	0.333%
48	7.182	1812	1817	1823	rBV3	946	884	0.10%	0.011%
49	7.282	1844	1848	1850	rBV2	307	280	0.03%	0.003%
50	7.514	1915	1920	1924	rBV	218	269	0.03%	0.003%
51	7.565	1924	1936	1956	rBV2	124121	219466	23.63%	2.719%
52	7.681	1963	1972	1974	rBV2	830	1044	0.11%	0.013%
53	7.777	1997	2002	2003	rBV	364	241	0.03%	0.003%
54	7.899	2025	2040	2056	rBV	430008	742024	79.89%	9.193%
55	8.179	2115	2127	2143	rBV2	89860	159852	17.21%	1.980%
56	8.472	2209	2218	2228	rBV4	3147	4983	0.54%	0.062%
57	8.555	2234	2244	2255	rBV3	14673	25335	2.73%	0.314%
58	8.632	2255	2268	2302	rBV	282625	521349	56.13%	6.459%
59	8.787	2305	2316	2345	rVB	219334	385298	41.48%	4.774%
60	8.919	2356	2357	2362	rVB	341	202	0.02%	0.003%
61	9.022	2386	2389	2394	rBV2	336	290	0.03%	0.004%
62	9.060	2397	2401	2404	rBV2	209	178	0.02%	0.002%
63	9.105	2411	2415	2419	rBV	326	371	0.04%	0.005%
64	9.144	2423	2427	2429	rBV	254	247	0.03%	0.003%
65	9.417	2498	2512	2531	rBV	432077	719664	77.49%	8.916%
66	9.578	2556	2562	2572	rVB3	725	1105	0.12%	0.014%
67	9.642	2572	2582	2585	rBV4	981	1488	0.16%	0.018%
68	9.700	2591	2600	2605	rVB2	1380	1821	0.20%	0.023%
69	9.890	2656	2659	2661	rBV	275	167	0.02%	0.002%
70	10.095	2721	2723	2728	rBV2	504	396	0.04%	0.005%
71	10.153	2738	2741	2743	rBV	323	205	0.02%	0.003%
72	10.237	2761	2767	2770	rBV2	905	794	0.09%	0.010%
73	10.346	2791	2801	2816	rVB4	21633	35915	3.87%	0.445%
74	10.485	2840	2844	2851	rBV	291	329	0.04%	0.004%
75	10.668	2897	2901	2906	rBV2	508	415	0.04%	0.005%
76	10.758	2916	2929	2951	rBV	314048	510366	54.95%	6.323%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051622\
 Data File : VU048589.D
 Acq On : 16 May 2022 18:47
 Operator : SY/MD
 Sample : N2849-01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXXW6

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % 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:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
 Title : VOC Analysis

77	10.893	2962	2971	2985	rVB3	3258	5519	0.59%	0.068%
78	10.967	2991	2994	3000	rVB2	223	216	0.02%	0.003%
79	11.092	3030	3033	3035	rBV	480	257	0.03%	0.003%
80	11.308	3093	3100	3107	rBV6	2355	3917	0.42%	0.049%
81	11.459	3143	3147	3149	rBV	740	646	0.07%	0.008%
82	11.581	3176	3185	3201	rVB4	4569	8378	0.90%	0.104%
83	11.645	3202	3205	3209	rBV	334	296	0.03%	0.004%
84	11.693	3212	3220	3231	rVB6	9293	13836	1.49%	0.171%
85	11.742	3233	3235	3241	rVB3	603	473	0.05%	0.006%
86	11.812	3245	3257	3274	rBV	484469	766819	82.56%	9.500%
87	12.066	3330	3336	3344	rVB6	2794	3945	0.42%	0.049%
88	12.195	3361	3376	3391	rBV	461243	747758	80.51%	9.264%
89	12.279	3400	3402	3405	rVB3	476	220	0.02%	0.003%
90	12.558	3484	3489	3499	rVB5	2354	3002	0.32%	0.037%
91	12.709	3534	3536	3537	rBV5	392	201	0.02%	0.002%
92	12.893	3586	3593	3602	rVB7	9168	13147	1.42%	0.163%
93	13.005	3625	3628	3631	rBV2	345	251	0.03%	0.003%
94	13.218	3689	3694	3706	rVB5	1977	2094	0.23%	0.026%
95	13.295	3716	3718	3720	rBV	403	266	0.03%	0.003%
96	13.356	3735	3737	3739	rBV	476	219	0.02%	0.003%
97	13.841	3886	3888	3889	rBV	836	343	0.04%	0.004%
98	13.928	3912	3915	3917	rBV	401	295	0.03%	0.004%
99	14.481	4085	4087	4090	rBV2	399	206	0.02%	0.003%
100	14.562	4110	4112	4116	rBV2	374	289	0.03%	0.004%

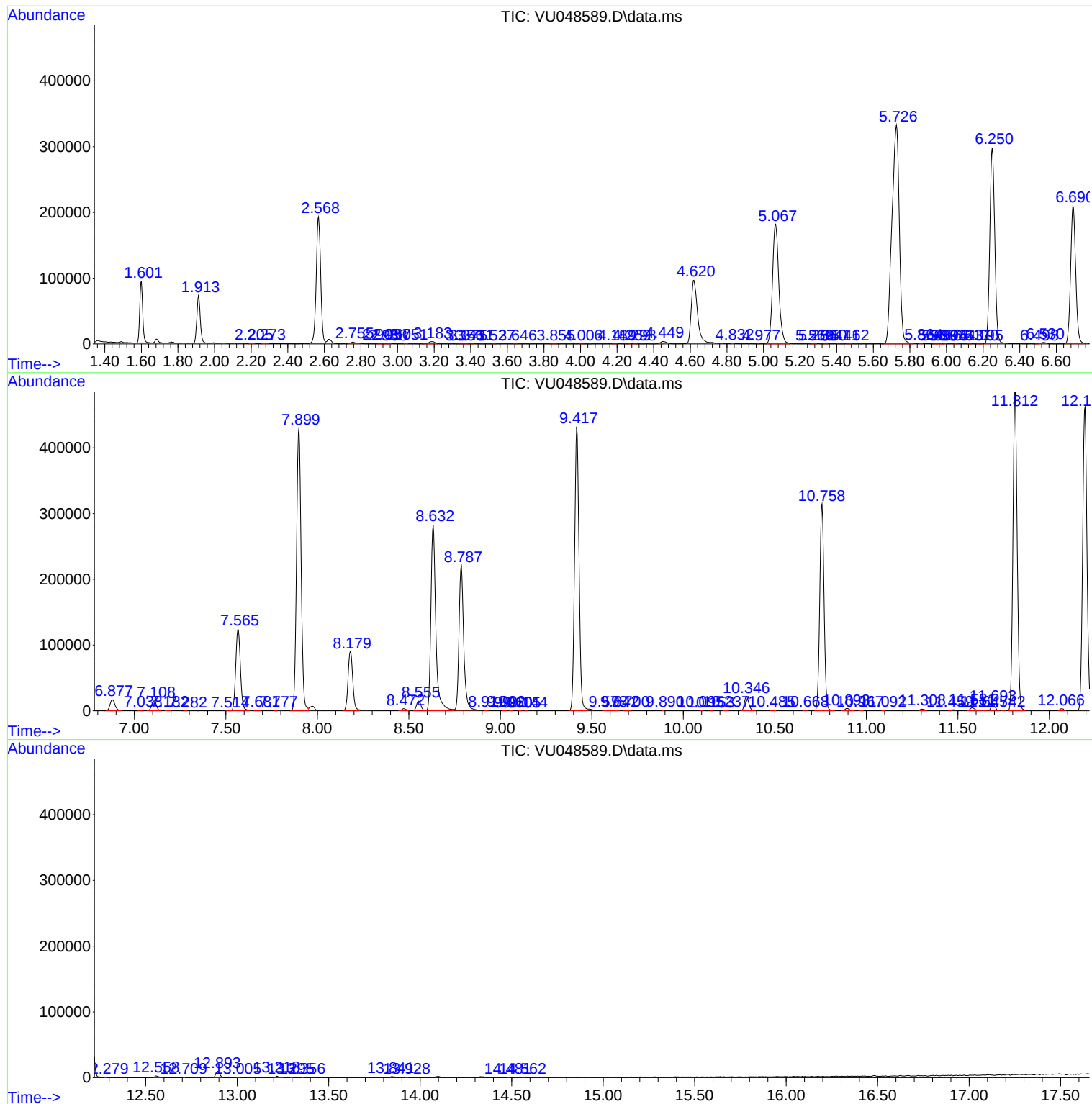
Sum of corrected areas: 8071539

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051622\
Data File : VU048589.D
Acq On : 16 May 2022 18:47
Operator : SY/MD
Sample : N2849-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXXW6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051622\
Data File : VU048589.D
Acq On : 16 May 2022 18:47
Operator : SY/MD
Sample : N2849-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXXW6

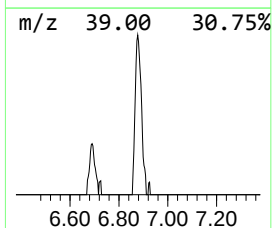
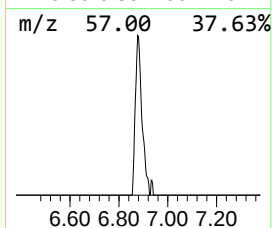
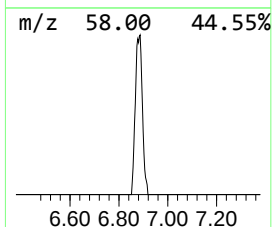
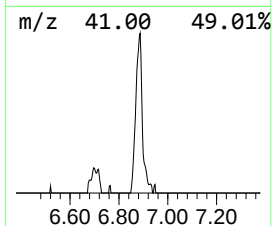
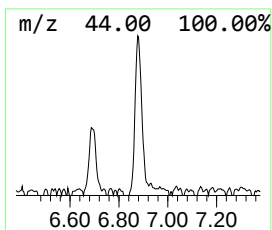
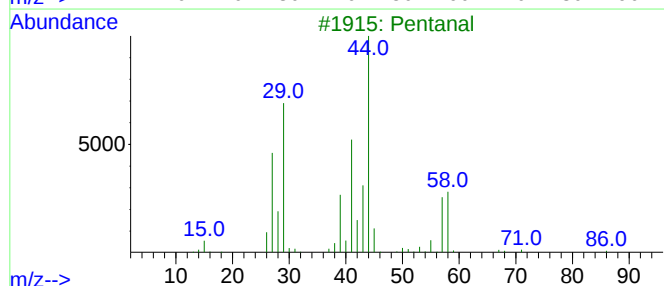
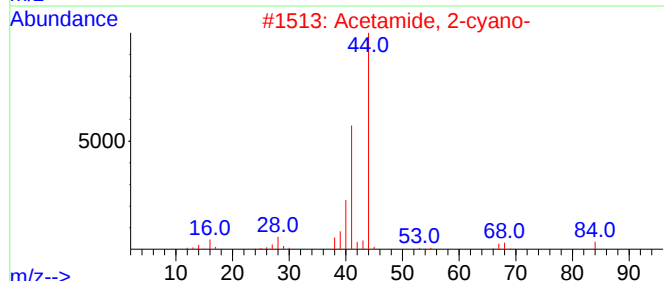
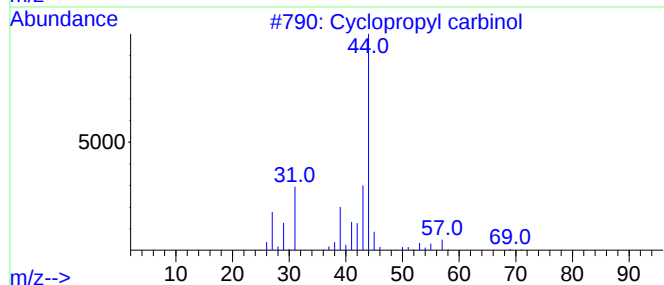
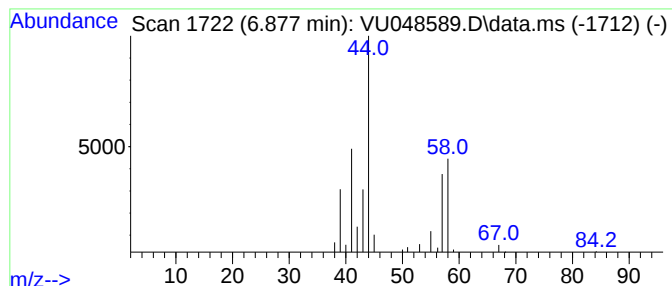
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.877	2.84 ug/L	32072	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropyl carbinol	72	C4H8O	002516-33-8	28
2			Acetamide, 2-cyano-	84	C3H4N2O	000107-91-5	23
3			Pentanal	86	C5H10O	000110-62-3	9
4			1-Octadecanamine, N-methyl-	283	C19H41N	002439-55-6	9
5			Cyclopropyl carbinol	72	C4H8O	002516-33-8	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051622\
Data File : VU048589.D
Acq On : 16 May 2022 18:47
Operator : SY/MD
Sample : N2849-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXXW6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	6.877	2.8	ug/L	32072	1	6.250	563748	50.0