

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082224\
 Data File : BG062555.D
 Acq On : 23 Aug 2024 1:32
 Operator : MA/JU
 Sample : P3673-19
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DCYI9

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF Filtering: 5
 Sampling : 1 Min Area: 0.1 % 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_G\Methods\SFAM-EPA-BG081424.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BG062555.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.402	15	19	24	rVB4	10159	14219	0.95%	0.075%
2	3.602	51	53	58	rVB4	3923	5353	0.36%	0.028%
3	3.661	60	63	71	rBV	38165	59895	4.00%	0.317%
4	3.808	84	88	99	rBV	67373	109490	7.31%	0.579%
5	4.143	143	145	149	rVB3	3447	4003	0.27%	0.021%
6	5.047	296	299	303	rBV3	2347	3865	0.26%	0.020%
7	5.893	438	443	444	rBV3	1195	2137	0.14%	0.011%
8	6.016	458	464	469	rBV	8567	15189	1.01%	0.080%
9	6.204	490	496	498	rBV4	2074	2604	0.17%	0.014%
10	6.633	565	569	574	rVB5	3089	4238	0.28%	0.022%
11	7.097	641	648	659	rBV	194755	331363	22.13%	1.754%
12	7.262	669	676	684	rBV	124617	204584	13.66%	1.083%
13	7.467	703	711	718	rBV	166581	278360	18.59%	1.473%
14	7.526	718	721	729	rVV2	7006	12257	0.82%	0.065%
15	7.937	783	791	797	rBV	270501	451282	30.14%	2.388%
16	8.002	797	802	807	rVB7	5604	9361	0.63%	0.050%
17	8.636	903	910	920	rBV	244586	410965	27.44%	2.175%
18	9.089	979	987	994	rVV	154914	273507	18.27%	1.447%
19	9.529	1056	1062	1067	rVB2	2526	4241	0.28%	0.022%
20	9.647	1076	1082	1090	rVB2	23816	38701	2.58%	0.205%
21	9.805	1102	1109	1120	rBV	135739	235731	15.74%	1.247%
22	10.346	1193	1201	1210	rBV	242416	416652	27.82%	2.205%
23	10.728	1258	1266	1274	rBV	414094	719280	48.03%	3.806%
24	10.857	1280	1288	1300	rBV	218471	395582	26.42%	2.093%
25	11.256	1351	1356	1363	rVB2	8463	14295	0.95%	0.076%
26	11.462	1385	1391	1399	rBV	40644	80960	5.41%	0.428%
27	12.308	1530	1535	1542	rVB	4503	7299	0.49%	0.039%
28	13.330	1706	1709	1714	rVB2	1893	2225	0.15%	0.012%
29	13.389	1714	1719	1725	rBV3	3909	6403	0.43%	0.034%
30	13.453	1725	1730	1735	rVB3	9614	14186	0.95%	0.075%
31	13.747	1774	1780	1783	rBV3	1416	2611	0.17%	0.014%
32	13.959	1810	1816	1823	rVV	444177	637265	42.56%	3.372%
33	14.205	1853	1858	1859	rBV2	5168	6729	0.45%	0.036%
34	14.246	1859	1865	1875	rVB	509039	786989	52.56%	4.165%
35	14.411	1889	1893	1896	rBV2	1560	2114	0.14%	0.011%
36	14.458	1899	1901	1906	rVB4	2511	3300	0.22%	0.017%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0.1 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
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37	14.558	1911	1918	1925	rBV	752670	1149165	76.74%	6.081%
38	14.628	1927	1930	1937	rVB6	6128	12910	0.86%	0.068%
39	14.758	1943	1952	1954	rBV4	410520	747683	49.93%	3.957%
40	14.781	1954	1956	1964	rVB	406882	447333	29.87%	2.367%
41	14.975	1984	1989	1993	rVB4	3096	5437	0.36%	0.029%
42	15.110	2009	2012	2016	rVB5	4144	5799	0.39%	0.031%
43	15.357	2049	2054	2058	rBV3	3531	6090	0.41%	0.032%
44	15.410	2058	2063	2068	rBV4	3524	4626	0.31%	0.024%
45	15.545	2080	2086	2093	rBV	681201	1042107	69.59%	5.515%
46	15.656	2099	2105	2114	rBV	185559	269744	18.01%	1.427%
47	15.786	2121	2127	2131	rBV5	3035	6090	0.41%	0.032%
48	15.921	2144	2150	2152	rBV2	1695	2425	0.16%	0.013%
49	15.979	2158	2160	2164	rVB3	2446	2965	0.20%	0.016%
50	16.103	2175	2181	2182	rBV3	3649	5071	0.34%	0.027%
51	16.179	2191	2194	2199	rVB3	3373	5460	0.36%	0.029%
52	16.273	2206	2210	2214	rBV3	5037	6491	0.43%	0.034%
53	16.314	2214	2217	2222	rVB4	2322	3747	0.25%	0.020%
54	16.444	2236	2239	2244	rVB5	2245	4238	0.28%	0.022%
55	16.696	2281	2282	2286	rBV3	2298	2366	0.16%	0.013%
56	16.808	2298	2301	2304	rVB3	1978	2316	0.15%	0.012%
57	16.855	2306	2309	2313	rBV5	5767	7040	0.47%	0.037%
58	17.019	2332	2337	2338	rBV5	2206	2518	0.17%	0.013%
59	17.049	2338	2342	2343	rBV4	4720	4660	0.31%	0.025%
60	17.219	2370	2371	2375	rVB4	1691	2058	0.14%	0.011%
61	17.301	2377	2385	2392	rVV	903446	1378419	92.05%	7.295%
62	17.395	2395	2401	2411	rVV	728338	1051436	70.22%	5.564%
63	17.489	2414	2417	2418	rVV3	2217	2247	0.15%	0.012%
64	17.806	2467	2471	2473	rVB4	2119	2624	0.18%	0.014%
65	17.830	2473	2475	2481	rVB2	1621	2333	0.16%	0.012%
66	17.971	2495	2499	2503	rVB4	9003	10723	0.72%	0.057%
67	18.059	2510	2514	2515	rBV2	3308	3076	0.21%	0.016%
68	18.194	2530	2537	2545	rBV	92118	160089	10.69%	0.847%
69	18.411	2572	2574	2578	rVB5	3525	3623	0.24%	0.019%
70	18.494	2585	2588	2589	rVV3	3264	3422	0.23%	0.018%
71	18.529	2591	2594	2600	rVB5	8080	14012	0.94%	0.074%
72	18.623	2606	2610	2613	rBV4	2509	3941	0.26%	0.021%
73	18.652	2613	2615	2617	rVV3	2441	2203	0.15%	0.012%
74	18.740	2628	2630	2634	rBV4	3317	2776	0.19%	0.015%
75	18.829	2639	2645	2646	rBV6	3341	4602	0.31%	0.024%
76	18.987	2670	2672	2675	rBV4	3210	3834	0.26%	0.020%

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77	19.058	2680	2684	2690	rVV8	6943	12185	0.81%	0.064%
78	19.140	2695	2698	2703	rVB4	17709	24273	1.62%	0.128%
79	19.251	2712	2717	2720	rBV5	9759	17618	1.18%	0.093%
80	19.316	2725	2728	2733	rBV	13254	20279	1.35%	0.107%
81	19.369	2735	2737	2746	rVB8	9549	21223	1.42%	0.112%
82	19.469	2748	2754	2758	rBV2	30015	47846	3.20%	0.253%
83	19.563	2765	2770	2773	rVB6	16455	24502	1.64%	0.130%
84	19.616	2773	2779	2784	rBV7	15153	25721	1.72%	0.136%
85	19.686	2784	2791	2796	rVV	833373	1229148	82.08%	6.505%
86	19.733	2796	2799	2804	rVB4	15092	21792	1.46%	0.115%
87	20.203	2877	2879	2881	rBV2	8443	7515	0.50%	0.040%
88	20.485	2925	2927	2932	rBV6	6423	12314	0.82%	0.065%
89	20.532	2932	2935	2936	rVV3	7846	8185	0.55%	0.043%
90	20.561	2938	2940	2945	rVB6	14336	18342	1.22%	0.097%
91	20.661	2954	2957	2961	rVB6	11279	12726	0.85%	0.067%
92	20.714	2962	2966	2970	rBV6	16213	28115	1.88%	0.149%
93	21.214	3047	3051	3058	rBV	125158	208687	13.94%	1.104%
94	21.542	3101	3107	3116	rVB2	842681	1353046	90.36%	7.160%
95	22.993	3352	3354	3361	rVB5	21507	35474	2.37%	0.188%
96	23.769	3480	3486	3492	rBV2	39029	74820	5.00%	0.396%
97	24.415	3586	3596	3607	rBV	447928	1151186	76.88%	6.092%
98	24.627	3622	3632	3647	rVB	543596	1497421	100.00%	7.924%
99	25.872	3835	3844	3862	rVB4	174051	605101	40.41%	3.202%
100	28.598	4297	4308	4325	rVB6	110599	474234	31.67%	2.510%

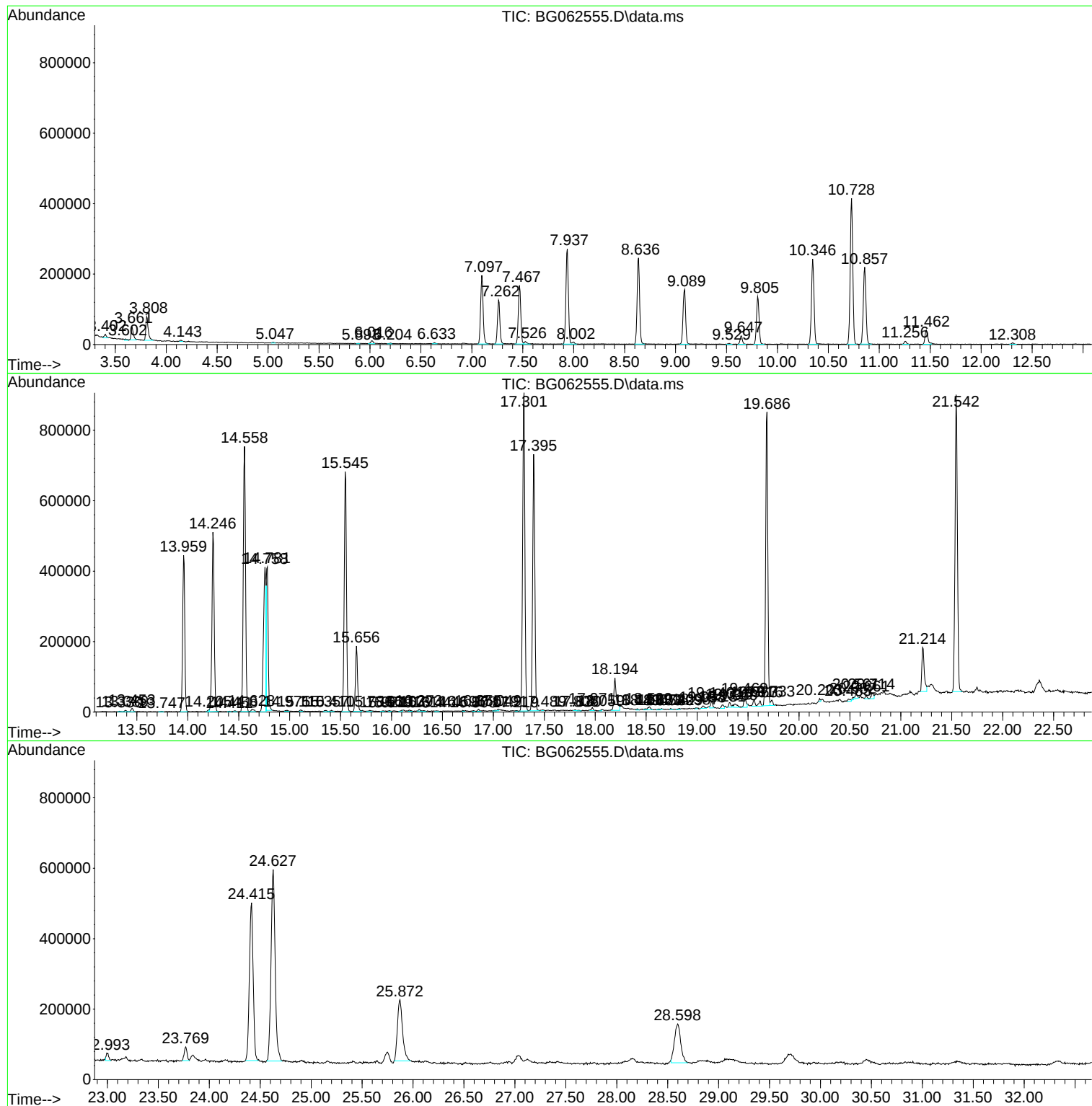
Sum of corrected areas: 18896687

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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



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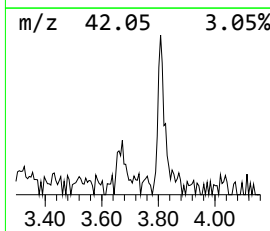
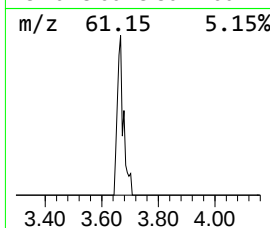
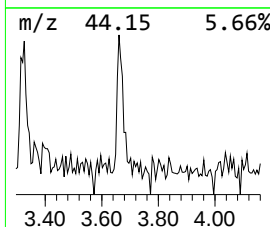
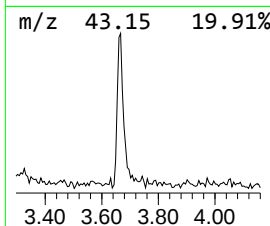
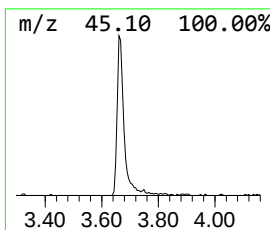
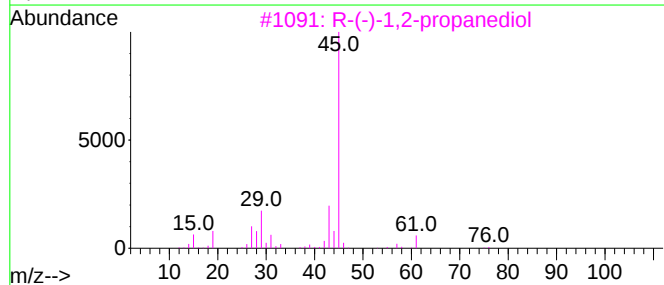
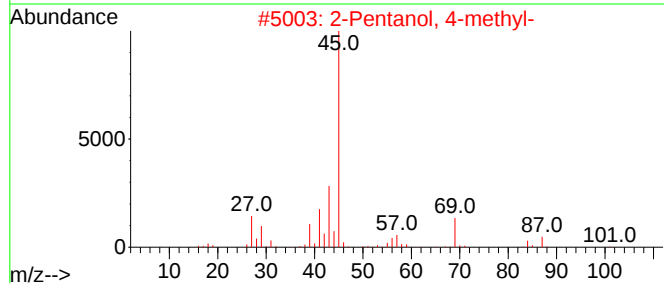
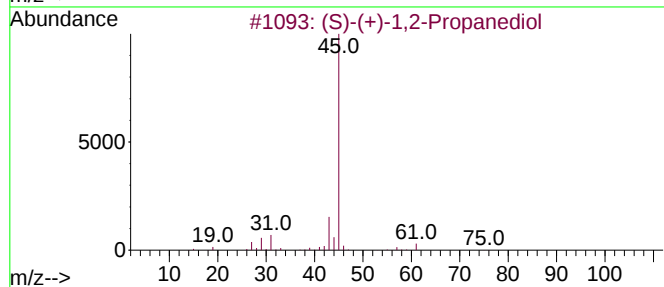
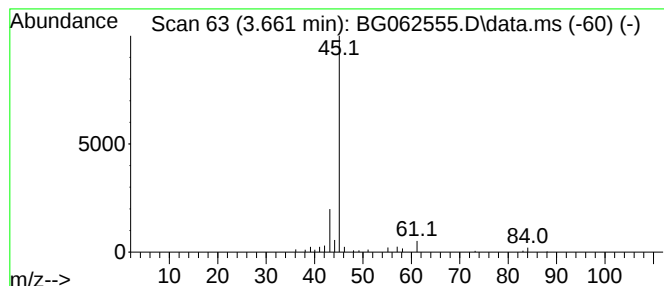
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.661	2.65 ng/ul	59895	1,4-Dichlorobenzene-d4	7.937

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	56
2	2-Pentanol, 4-methyl-			102	C6H14O	000108-11-2	40
3	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	40
4	Propylene Glycol			76	C3H8O2	000057-55-6	40
5	2-Hexanol, (R)-			102	C6H14O	026549-24-6	39



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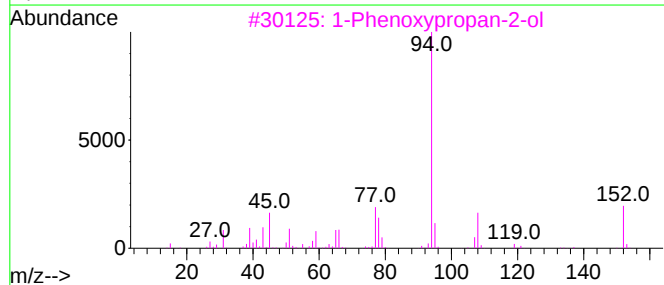
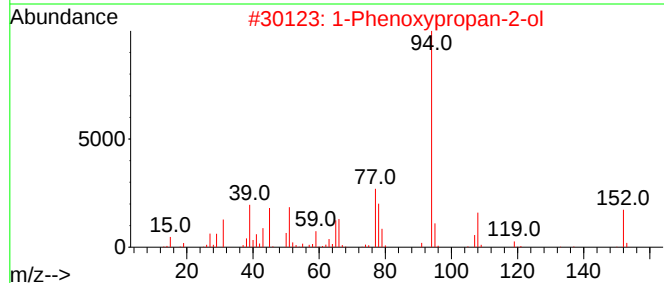
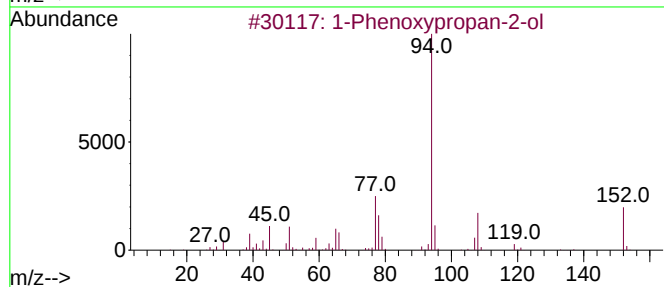
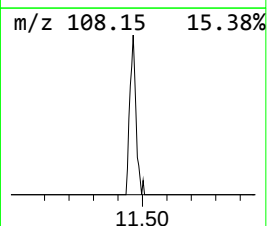
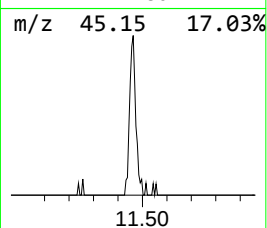
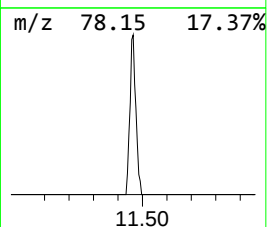
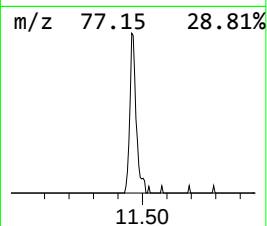
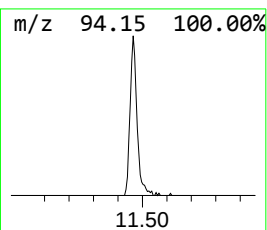
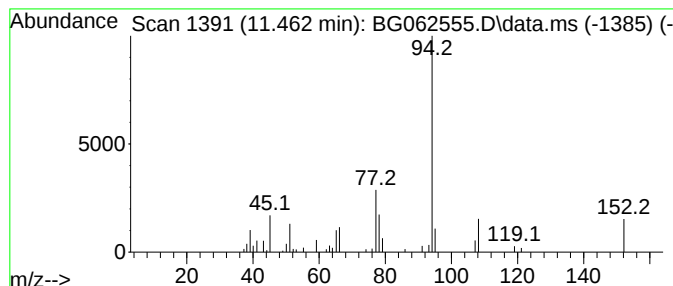
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.462	2.25 ng/ul	80960	Naphthalene-d8	10.728

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
3			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	87
4			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	87
5			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	59



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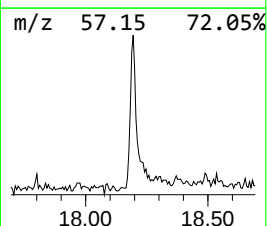
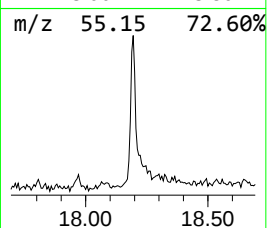
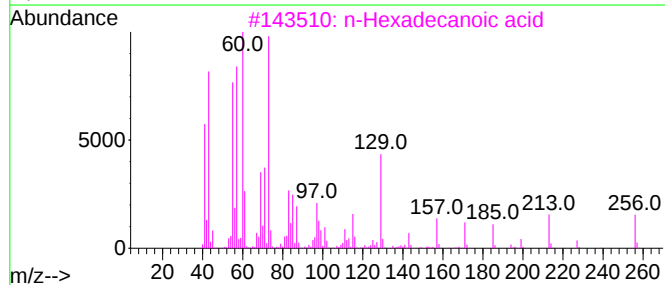
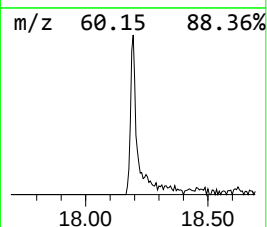
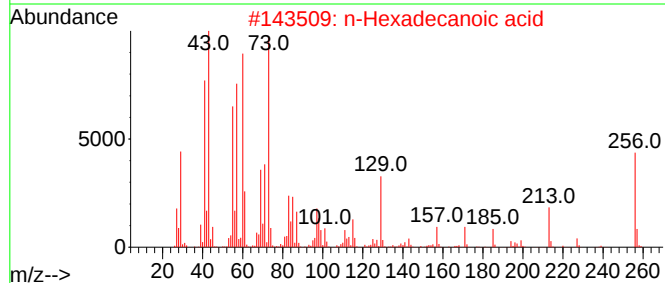
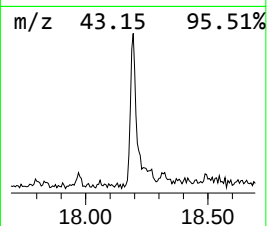
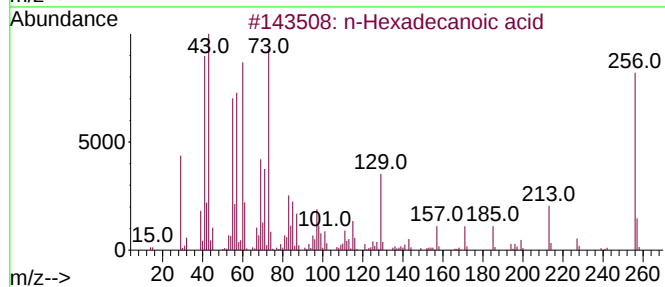
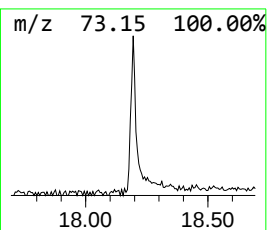
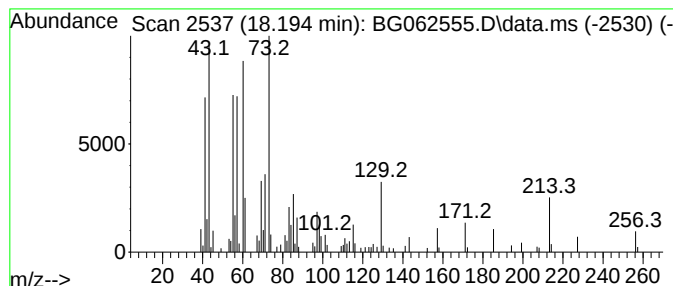
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.194	2.32 ng/ul	160089	Phenanthrene-d10	17.301

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
4			Tridecanoic acid	214	C13H26O2	000638-53-9	81
5			Tridecanoic acid	214	C13H26O2	000638-53-9	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082224\
Data File : BG062555.D
Acq On : 23 Aug 2024 1:32
Operator : MA/JU
Sample : P3673-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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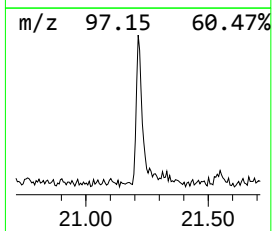
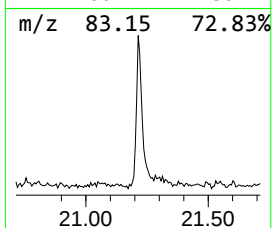
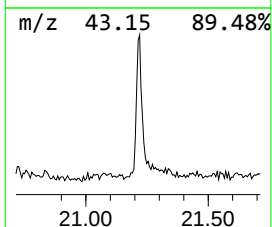
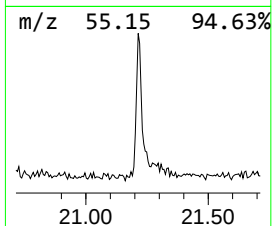
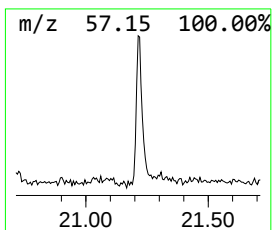
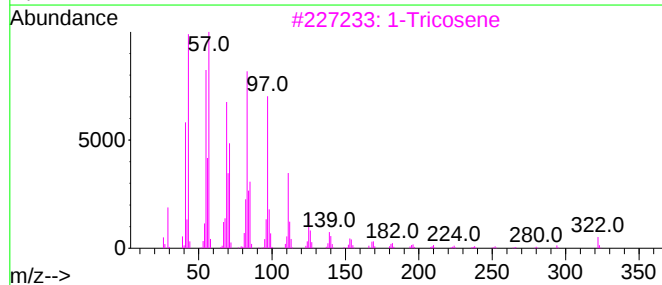
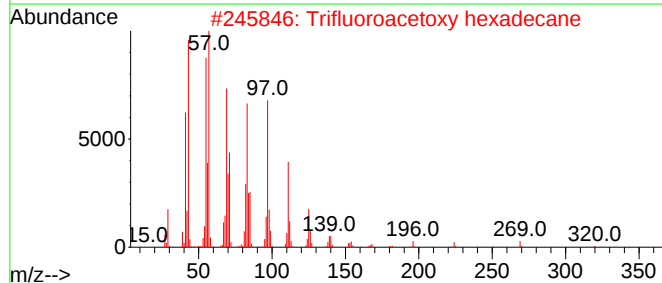
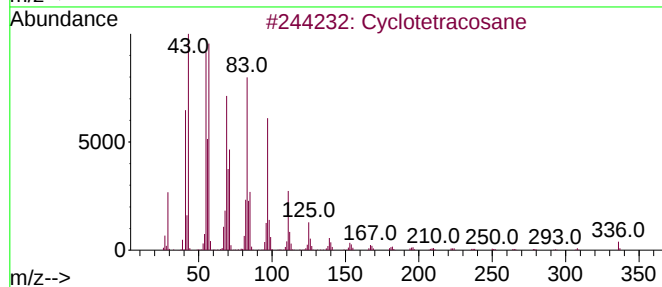
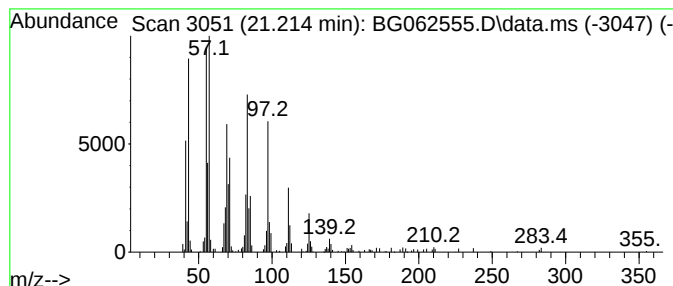
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 (DEL) Alkane: Cyclic21.214 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.214	3.08 ng/ul	208687	Chrysene-d12	21.543

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetracosane	336	C24H48	000297-03-0	95
2			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3			1-Tricosene	322	C23H46	018835-32-0	91
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082224\
Data File : BG062555.D
Acq On : 23 Aug 2024 1:32
Operator : MA/JU
Sample : P3673-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYI9

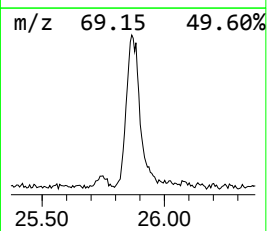
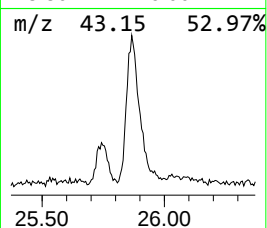
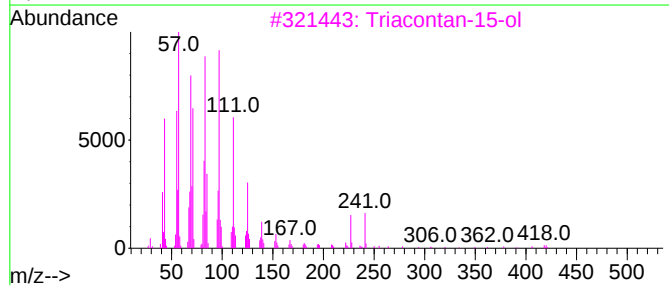
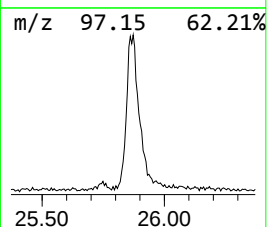
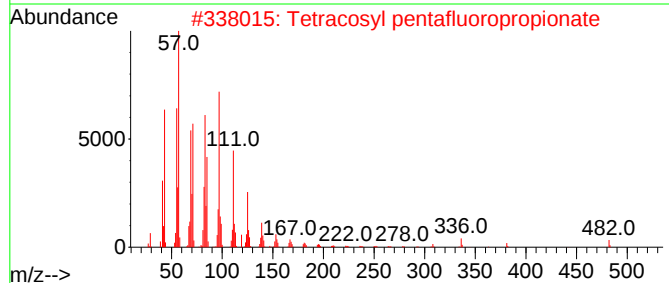
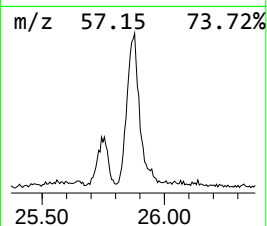
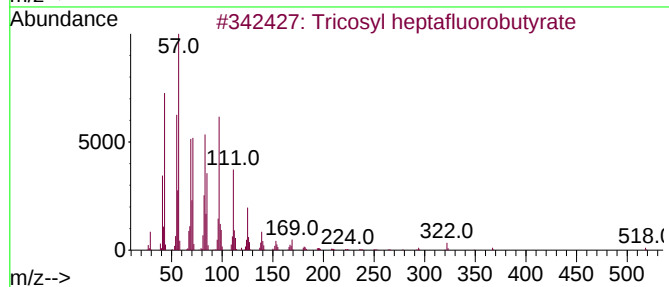
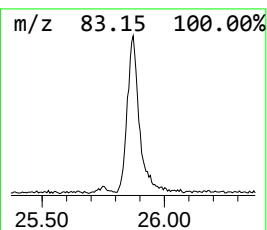
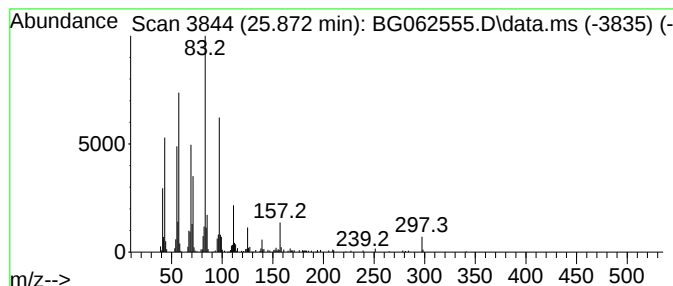
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.872	8.08 ng/ul	605101	Perylene-d12	24.627

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	45
2			Tetracosyl pentafluoropropionate	500	C27H49F5O2	1000351-81-3	43
3			Triacontan-15-ol	438	C30H62O	031849-26-0	38
4			Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	38
5			17-Pentatriacontene	491	C35H70	006971-40-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082224\
Data File : BG062555.D
Acq On : 23 Aug 2024 1:32
Operator : MA/JU
Sample : P3673-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYI9

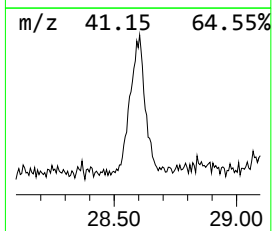
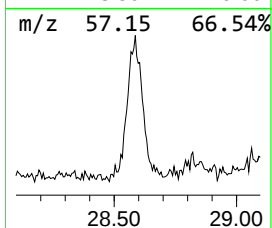
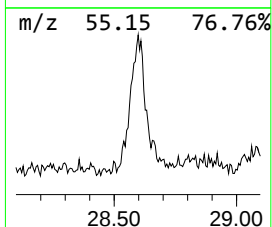
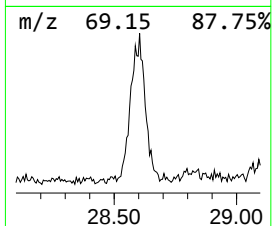
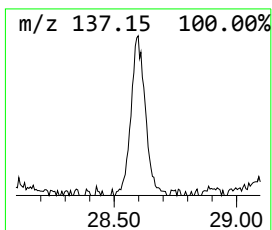
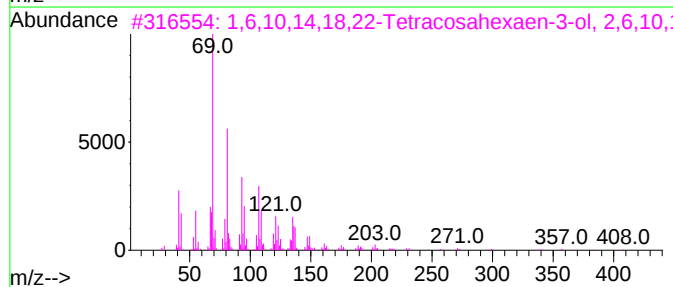
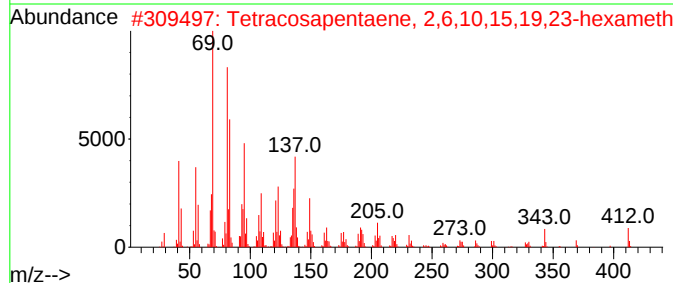
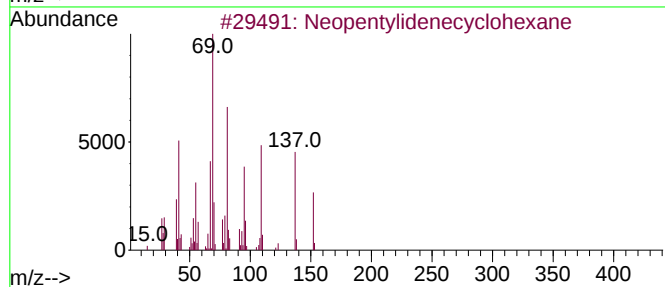
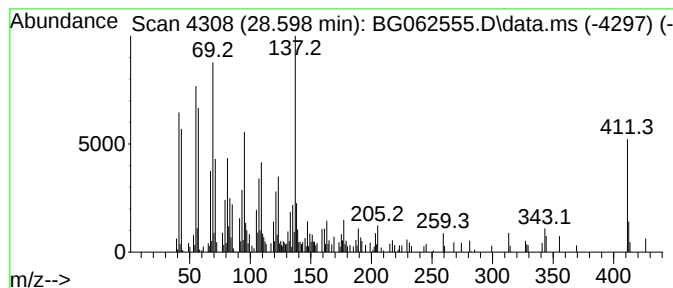
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.598	6.33 ng/ul	474234	Perylene-d12	24.627

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Neopentylidenecyclohexane	152	C11H20	039546-80-0	43
2			Tetracosapentaene, 2,6,10,15,19,...	412	C30H52	026266-08-0	38
3			1,6,10,14,18,22-Tetracosahexaen-...	426	C30H50O	097232-74-1	27
4			1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	27
5			VII tropolone	137	C7H7NO2	007021-46-7	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082224\
Data File : BG062555.D
Acq On : 23 Aug 2024 1:32
Operator : MA/JU
Sample : P3673-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYI9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(S)-(+)-1,2-Pro...	3.661	2.6	ng/ul	59895	1	7.937	451282	20.0
1-Phenoxypropan...	11.462	2.3	ng/ul	80960	2	10.728	719280	20.0
n-Hexadecanoic ...	18.194	2.3	ng/ul	160089	4	17.301	1378420	20.0
(DEL) Alkane: C...	21.214	3.1	ng/ul	208687	5	21.543	1353050	20.0
unknown-01	25.872	8.1	ng/ul	605101	6	24.627	1497420	20.0
unknown-02	28.598	6.3	ng/ul	474234	6	24.627	1497420	20.0