

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
 Data File : BG062338.D
 Acq On : 8 Aug 2024 20:56
 Operator : MA/JU
 Sample : P3434-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 E05T4

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-BG080524.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BG062338.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.334	6	8	13	rVB5	3487	4801	0.20%	0.018%
2	3.422	19	23	30	rVB	11379	17306	0.74%	0.066%
3	3.681	63	67	78	rVB	36646	59446	2.53%	0.228%
4	3.822	87	91	104	rBV	173998	293180	12.49%	1.123%
5	4.162	147	149	155	rVB3	3261	4562	0.19%	0.017%
6	6.042	464	469	477	rBV	12385	20108	0.86%	0.077%
7	7.111	644	651	661	rVB	262943	460082	19.60%	1.762%
8	7.288	672	681	689	rBV	181958	310050	13.21%	1.188%
9	7.487	708	715	721	rBV	241373	406158	17.30%	1.556%
10	7.546	721	725	730	rVB	10657	16142	0.69%	0.062%
11	7.957	788	795	801	rBV	237051	411987	17.55%	1.578%
12	8.016	801	805	811	rVB3	9257	14810	0.63%	0.057%
13	8.650	904	913	922	rBV	336193	561253	23.91%	2.150%
14	9.109	984	991	1001	rVB	252366	448012	19.08%	1.716%
15	9.667	1080	1086	1095	rBV	41219	64597	2.75%	0.247%
16	9.825	1106	1113	1121	rBV	209630	370905	15.80%	1.421%
17	10.360	1197	1204	1213	rBV	359582	644687	27.46%	2.469%
18	10.748	1262	1270	1278	rBV	387333	683948	29.13%	2.620%
19	10.877	1284	1292	1302	rBV	362811	648667	27.63%	2.485%
20	11.282	1355	1361	1366	rBV2	15244	24059	1.02%	0.092%
21	11.482	1386	1395	1408	rBV	66116	117445	5.00%	0.450%
22	12.234	1517	1523	1527	rVB4	2607	4833	0.21%	0.019%
23	12.328	1534	1539	1544	rBV	7628	11924	0.51%	0.046%
24	13.415	1718	1724	1731	rBV3	4278	7767	0.33%	0.030%
25	13.984	1814	1821	1827	rBV	697775	1038758	44.24%	3.979%
26	14.266	1857	1869	1878	rBV	847373	1322135	56.31%	5.064%
27	14.484	1902	1906	1911	rVV3	3706	5278	0.22%	0.020%
28	14.572	1914	1921	1929	rVB	676458	1067704	45.48%	4.090%
29	14.748	1944	1951	1955	rBV	276621	447085	19.04%	1.712%
30	14.783	1955	1957	1958	rVV	11537	13339	0.57%	0.051%
31	14.983	1986	1991	2001	rBV3	8095	13022	0.55%	0.050%
32	15.312	2042	2047	2051	rBV3	4403	6254	0.27%	0.024%
33	15.377	2054	2058	2063	rBV4	4878	7729	0.33%	0.030%
34	15.435	2063	2068	2072	rVV2	4543	5380	0.23%	0.021%
35	15.565	2083	2090	2098	rBV	1135351	1696970	72.28%	6.500%
36	15.670	2100	2108	2116	rBV	225725	340529	14.50%	1.304%

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37	15.729	2116	2118	2126	rVB3	4601	8679	0.37%	0.033%
38	15.805	2129	2131	2135	rVB4	3126	3704	0.16%	0.014%
39	16.117	2179	2184	2188	rBV3	4815	7320	0.31%	0.028%
40	16.293	2209	2214	2218	rBV2	5929	9770	0.42%	0.037%

41	16.722	2283	2287	2289	rBV2	3240	3899	0.17%	0.015%
42	17.092	2347	2350	2353	rVV4	6616	7913	0.34%	0.030%
43	17.121	2353	2355	2360	rVV4	2841	3980	0.17%	0.015%
44	17.215	2368	2371	2375	rVV4	9767	14416	0.61%	0.055%
45	17.309	2379	2387	2394	rVV	846615	1275675	54.33%	4.886%

46	17.356	2394	2395	2398	rVV	10264	7444	0.32%	0.029%
47	17.409	2398	2404	2413	rVV	1138335	1750868	74.57%	6.706%
48	17.497	2413	2419	2426	rVB5	8505	13572	0.58%	0.052%
49	17.744	2458	2461	2465	rVB	6332	7813	0.33%	0.030%
50	17.979	2497	2501	2509	rVB4	19323	34472	1.47%	0.132%

51	18.091	2513	2520	2525	rBV3	13346	22979	0.98%	0.088%
52	18.149	2526	2530	2536	rBV3	17493	27184	1.16%	0.104%
53	18.214	2536	2541	2556	rVV	266748	404659	17.24%	1.550%
54	18.514	2588	2592	2598	rBV6	9786	20298	0.86%	0.078%
55	18.649	2610	2615	2617	rBV5	3126	3606	0.15%	0.014%

56	18.684	2617	2621	2625	rVV4	6115	7982	0.34%	0.031%
57	18.754	2630	2633	2640	rBV8	3633	7013	0.30%	0.027%
58	18.878	2651	2654	2660	rBV5	4070	7073	0.30%	0.027%
59	19.007	2674	2676	2683	rVB4	2793	3918	0.17%	0.015%
60	19.089	2683	2690	2695	rVV7	14012	25382	1.08%	0.097%

61	19.136	2695	2698	2699	rVV3	6400	6657	0.28%	0.025%
62	19.160	2699	2702	2707	rVB6	8752	12466	0.53%	0.048%
63	19.260	2713	2719	2724	rBV2	17976	25701	1.09%	0.098%
64	19.330	2726	2731	2734	rVV2	28772	48546	2.07%	0.186%
65	19.359	2734	2736	2748	rVB3	35660	67947	2.89%	0.260%

66	19.483	2753	2757	2766	rBV2	70981	103782	4.42%	0.398%
67	19.641	2780	2784	2786	rVB5	7375	8580	0.37%	0.033%
68	19.694	2786	2793	2801	rBV	1478430	2162709	92.12%	8.284%
69	19.753	2801	2803	2806	rVB3	13102	14156	0.60%	0.054%
70	19.888	2824	2826	2830	rVB3	9263	9410	0.40%	0.036%

71	20.211	2878	2881	2885	rBV5	8807	11455	0.49%	0.044%
72	20.246	2885	2887	2891	rVB5	6495	6610	0.28%	0.025%
73	20.458	2919	2923	2930	rBV4	15720	22290	0.95%	0.085%
74	20.681	2957	2961	2963	rBV4	6523	7663	0.33%	0.029%
75	20.716	2965	2967	2968	rVV2	6190	4931	0.21%	0.019%

76	20.746	2970	2972	2975	rVV4	8946	10396	0.44%	0.040%
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77	20.775	2975	2977	2981	rVB4	9452	10496	0.45%	0.040%
78	20.922	2997	3002	3006	rBV2	31919	38046	1.62%	0.146%
79	21.227	3049	3054	3062	rVV2	140328	214163	9.12%	0.820%
80	21.462	3093	3094	3099	rVB4	6863	7649	0.33%	0.029%
81	21.551	3102	3109	3116	rBV2	907109	1457524	62.08%	5.583%
82	21.774	3143	3147	3151	rBV5	14224	18605	0.79%	0.071%
83	22.003	3183	3186	3195	rVB7	14161	20549	0.88%	0.079%
84	22.373	3244	3249	3255	rBV4	22374	45029	1.92%	0.172%
85	22.714	3305	3307	3309	rBV3	3838	4065	0.17%	0.016%
86	23.043	3358	3363	3368	rVB4	16465	27316	1.16%	0.105%
87	23.219	3389	3393	3399	rVV4	12380	22730	0.97%	0.087%
88	23.818	3489	3495	3500	rBV5	28424	60323	2.57%	0.231%
89	24.188	3554	3558	3564	rBV10	3924	7728	0.33%	0.030%
90	24.347	3579	3585	3586	rBV6	7654	13343	0.57%	0.051%
91	24.429	3588	3599	3616	rVB	879049	2347833	100.00%	8.993%
92	24.635	3624	3634	3644	rBV	567637	1545574	65.83%	5.920%
93	24.729	3646	3650	3659	rVB4	25480	60180	2.56%	0.231%
94	25.586	3794	3796	3798	rBV3	3351	3592	0.15%	0.014%
95	25.821	3827	3836	3846	rBV3	29057	92996	3.96%	0.356%
96	25.933	3846	3855	3863	rBV3	15595	51885	2.21%	0.199%
97	27.131	4052	4059	4070	rVB4	19399	63777	2.72%	0.244%
98	28.688	4302	4324	4338	rBV4	157383	990303	42.18%	3.793%
99	29.134	4386	4400	4421	rVB7	267833	1206806	51.40%	4.622%
100	29.892	4523	4529	4530	rBV6	16311	23687	1.01%	0.091%

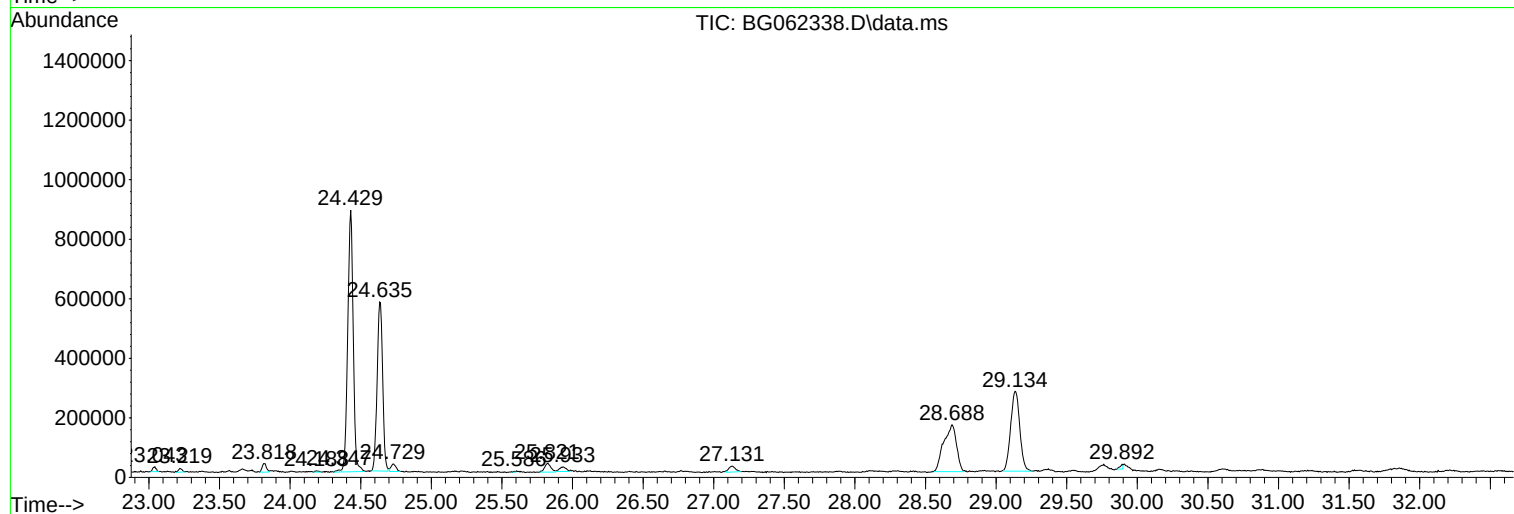
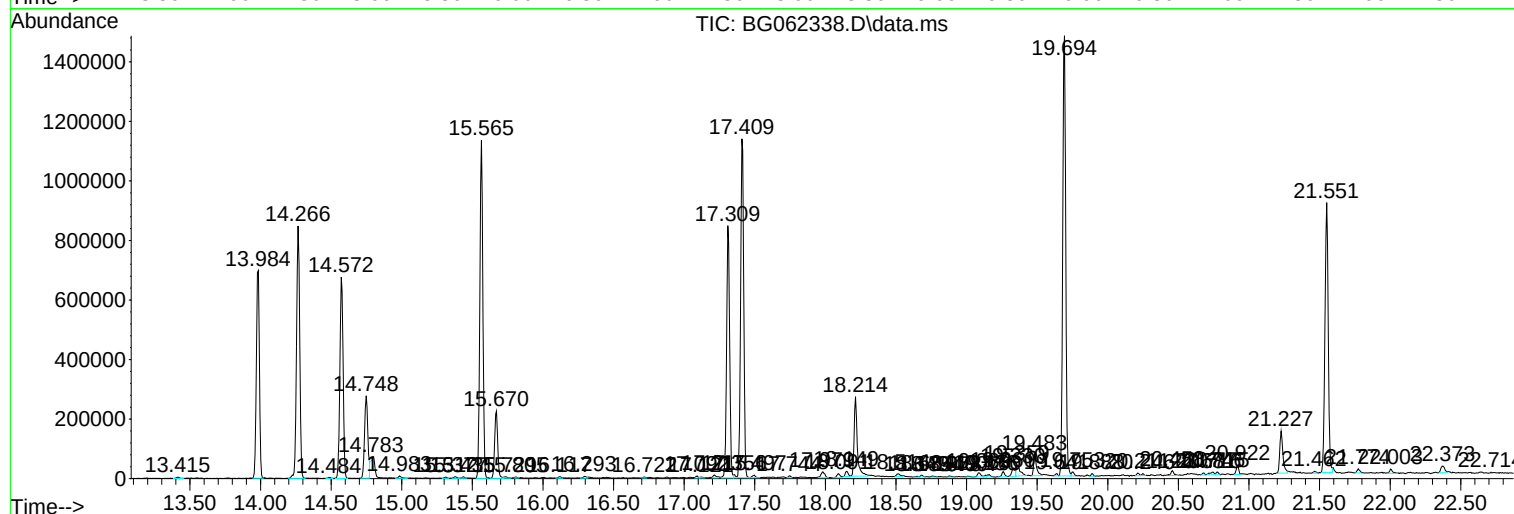
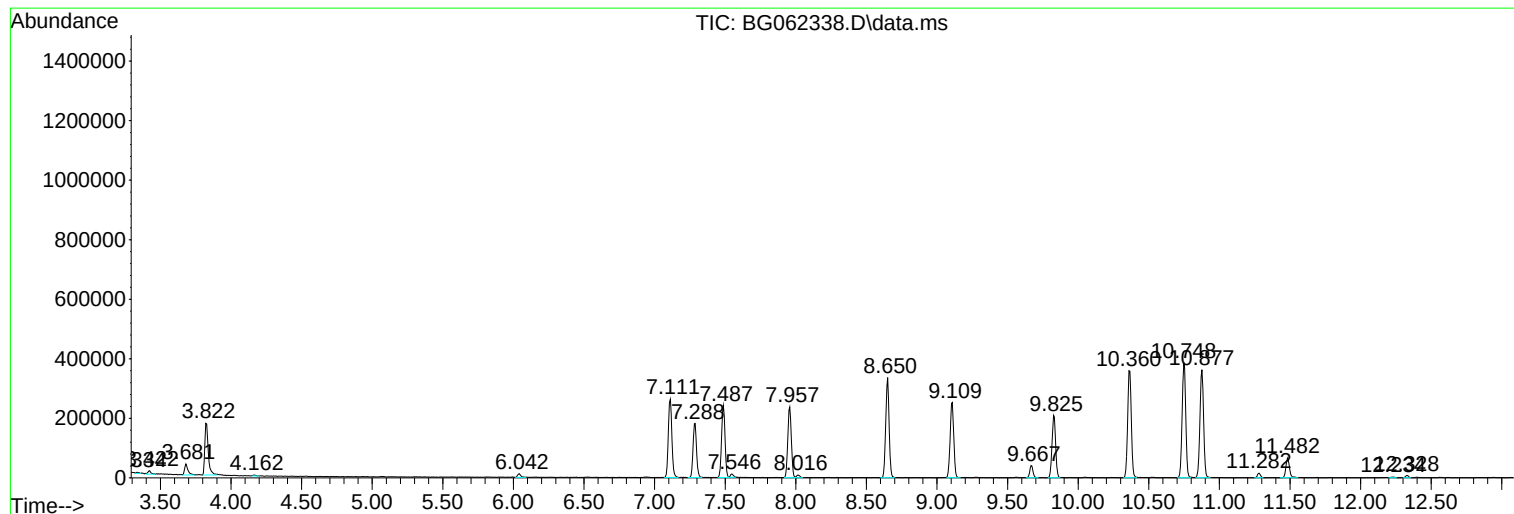
Sum of corrected areas: 26108029

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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

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



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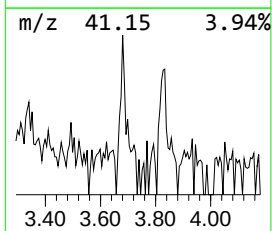
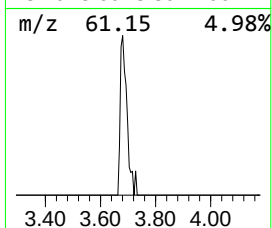
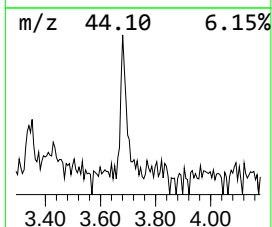
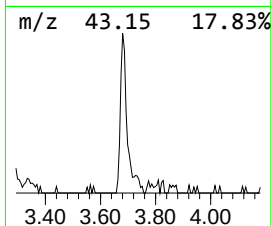
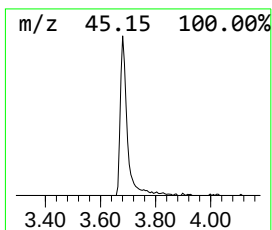
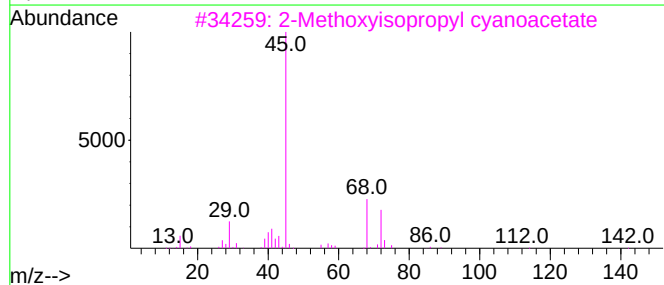
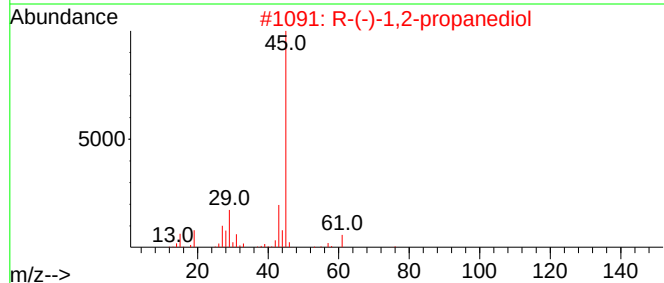
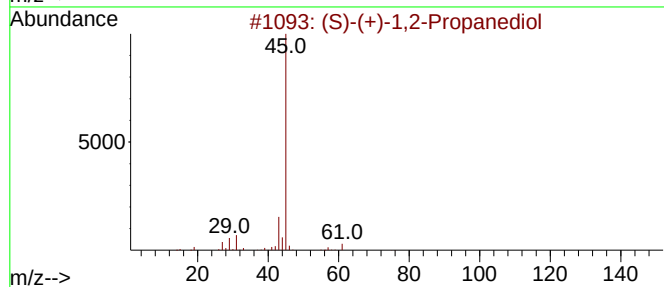
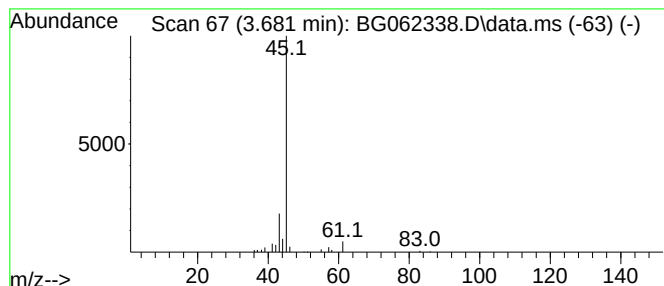
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.681	2.89 ng/ul	59446	1,4-Dichlorobenzene-d4	7.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	64
2	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	43
3	2-Methoxyisopropyl cyanoacetate			157	C7H11NO3	032804-79-8	9
4	Propylene Glycol			76	C3H8O2	000057-55-6	9
5	Propylene Glycol			76	C3H8O2	000057-55-6	9



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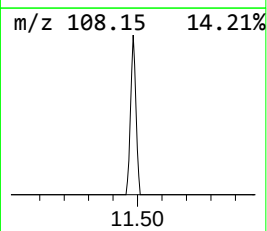
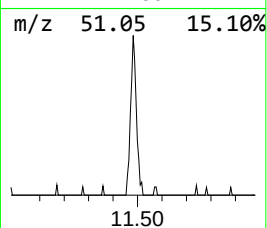
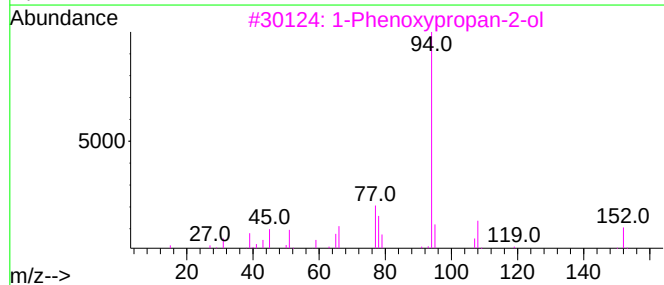
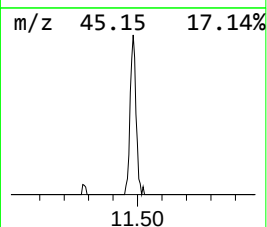
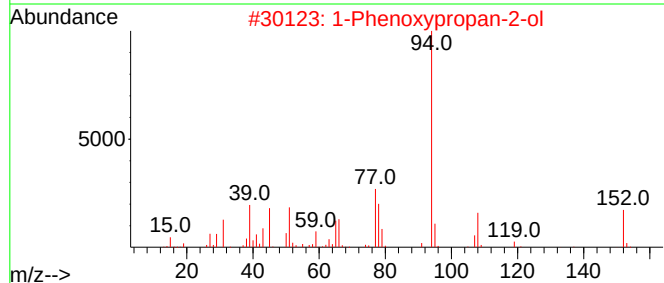
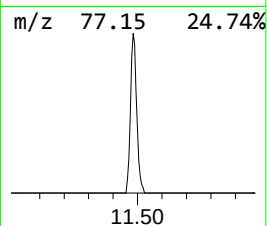
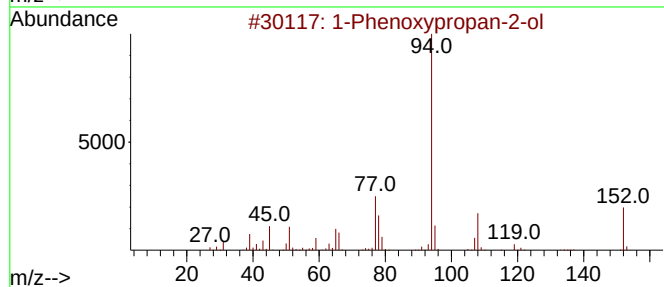
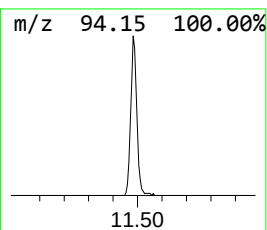
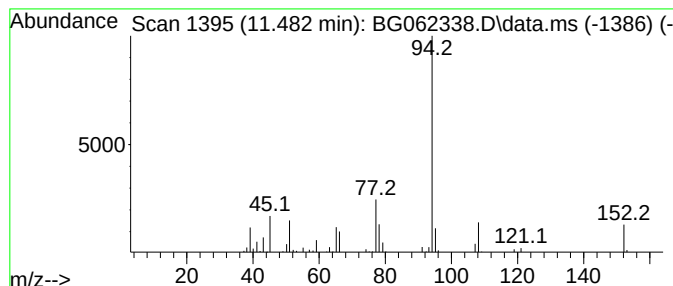
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.482	3.43 ng/ul	117445	Naphthalene-d8	10.748

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol		152	C9H12O2	000770-35-4	95	
2	1-Phenoxypropan-2-ol		152	C9H12O2	000770-35-4	94	
3	1-Phenoxypropan-2-ol		152	C9H12O2	000770-35-4	94	
4	1-Propanol, 3-phenoxy-		152	C9H12O2	006180-61-6	91	
5	Ethanol, 2-phenoxy-		138	C8H10O2	000122-99-6	64	



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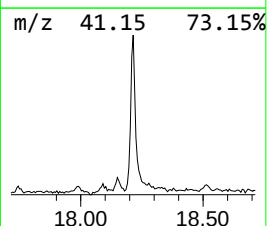
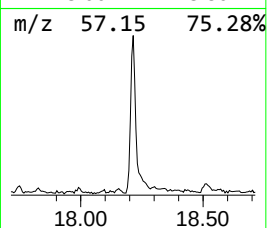
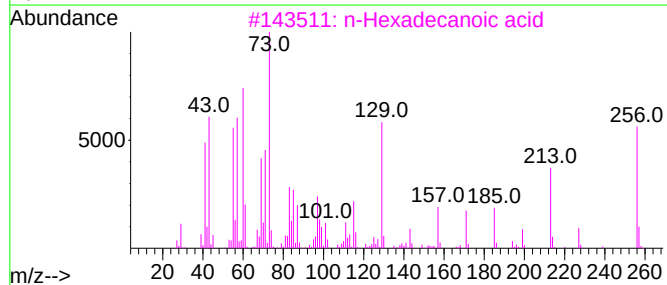
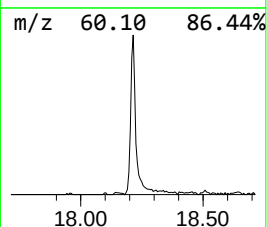
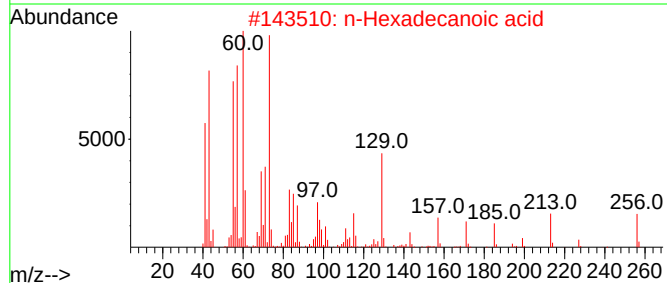
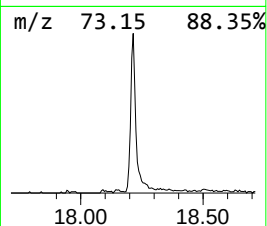
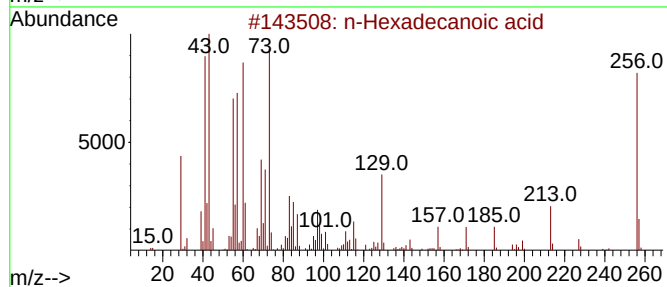
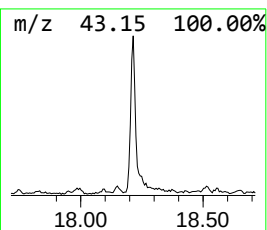
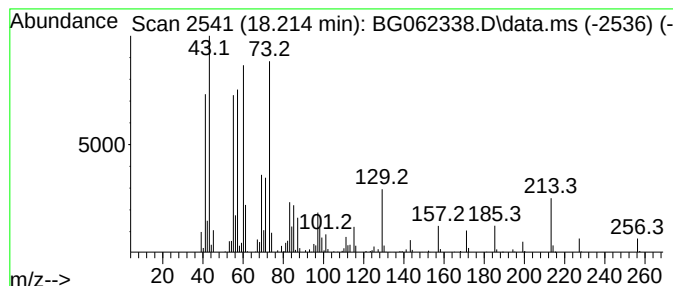
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.214	6.34 ng/ul	404659	Phenanthrene-d10	17.309

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	94
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062338.D
Acq On : 8 Aug 2024 20:56
Operator : MA/JU
Sample : P3434-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E05T4

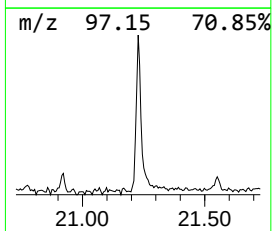
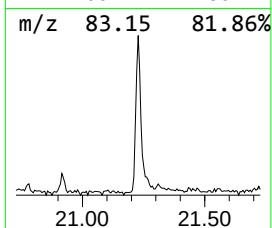
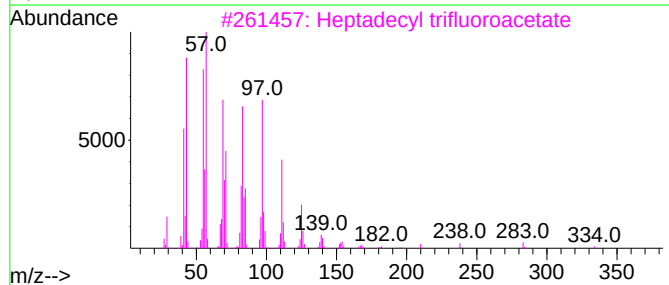
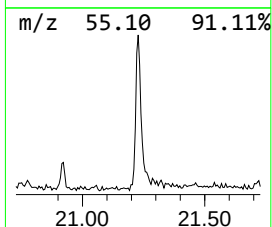
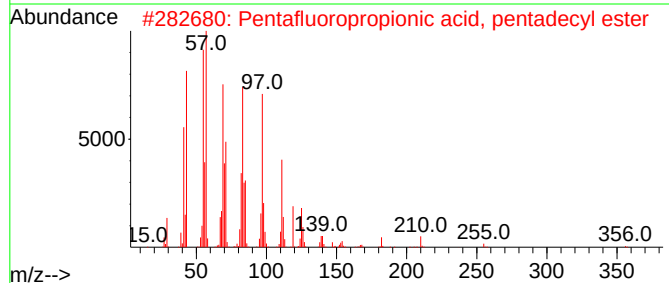
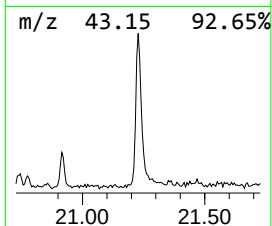
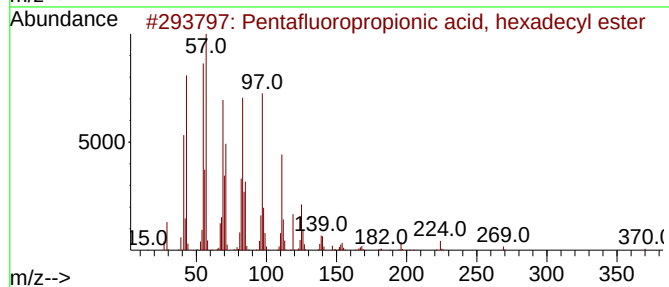
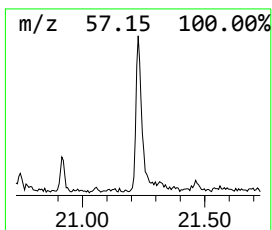
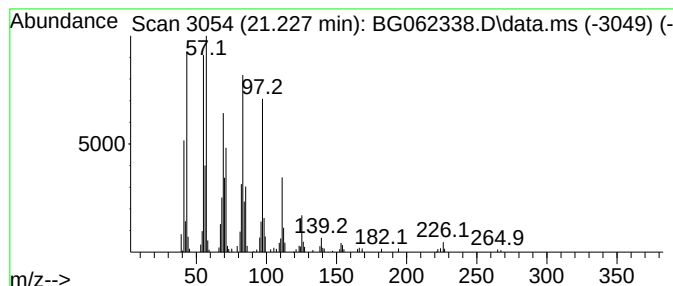
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.227	2.94 ng/ul	214163	Chrysene-d12	21.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
2			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
4			Behenic alcohol	326	C22H46O	000661-19-8	93
5			1-Heneicosanol	312	C21H44O	015594-90-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062338.D
Acq On : 8 Aug 2024 20:56
Operator : MA/JU
Sample : P3434-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E05T4

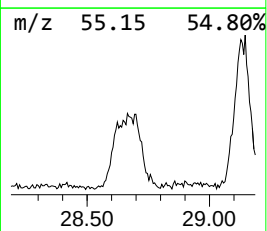
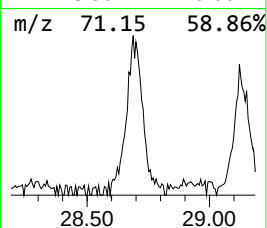
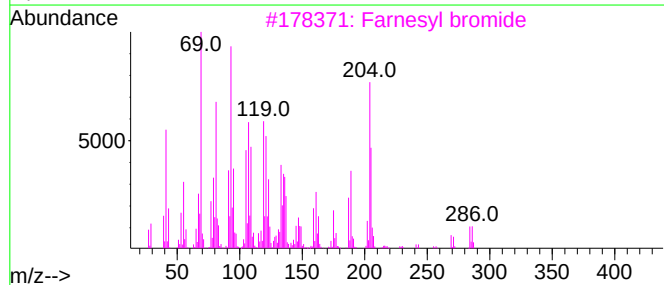
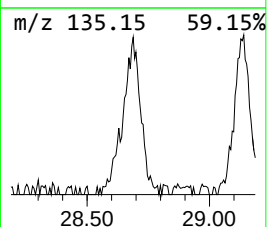
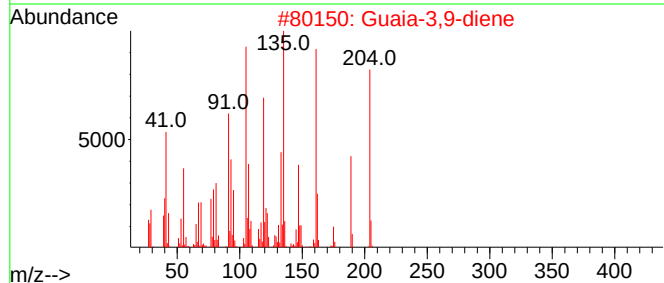
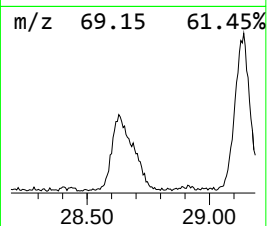
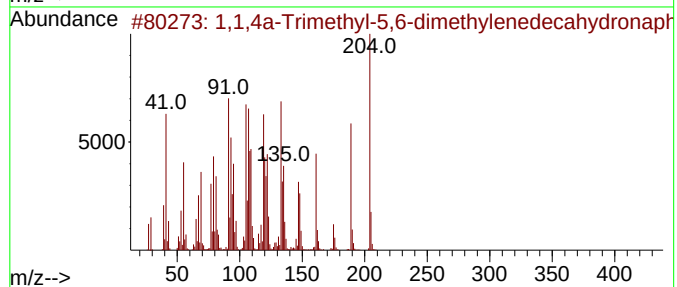
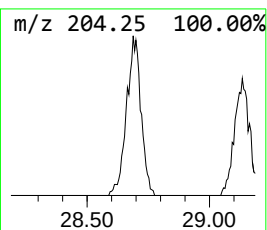
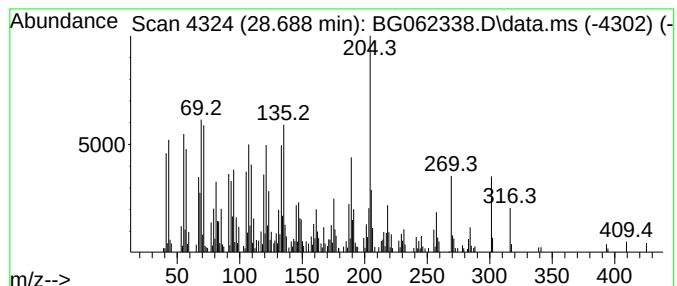
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 1,1,4a-Trimethyl-5,6-dimeth... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.688	12.81 ng/ul	990303	Perylene-d12	24.635

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	72		
2	Guaia-3,9-diene	204	C15H24	000489-83-8	58		
3	Farnesyl bromide	284	C15H25Br	006874-67-5	55		
4	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	52		
5	1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	49		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062338.D
Acq On : 8 Aug 2024 20:56
Operator : MA/JU
Sample : P3434-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E05T4

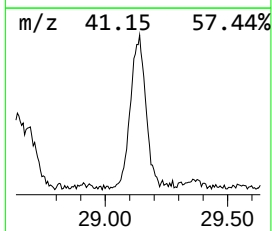
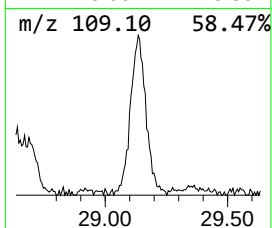
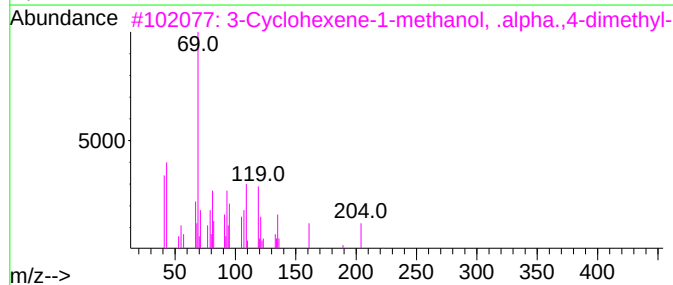
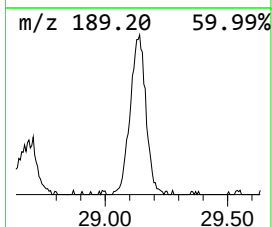
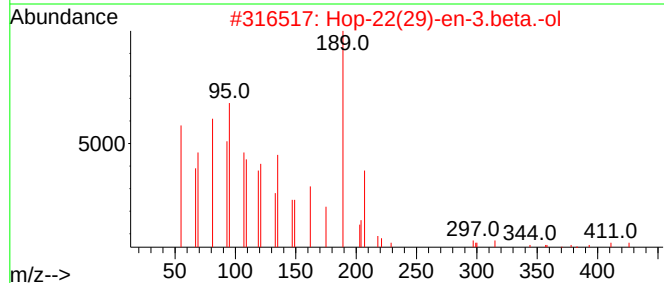
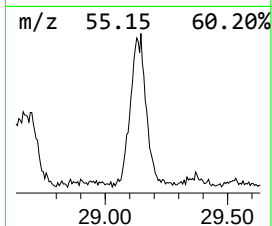
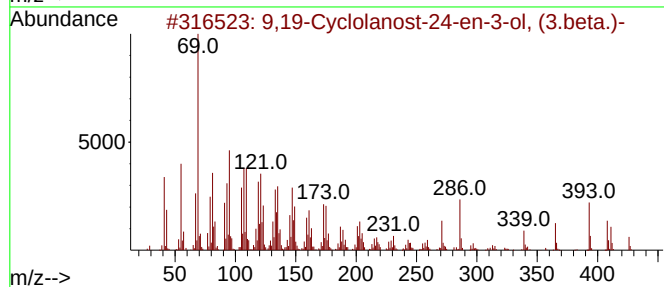
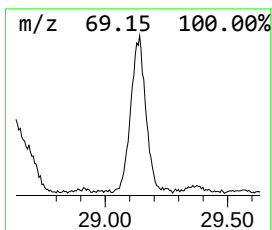
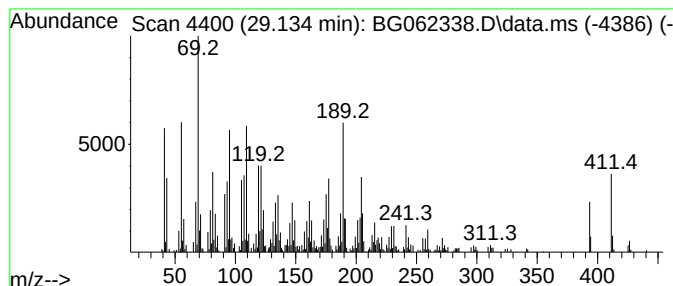
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 9,19-Cyclolanost-24-en-3-ol... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.134	15.62 ng/ul	1206810	Perylene-d12	24.635

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,19-Cyclolanost-24-en-3-ol, (3...	426	C30H50O	000469-38-5	95		
2	Hop-22(29)-en-3.beta.-ol	426	C30H50O	058801-23-3	60		
3	3-Cyclohexene-1-methanol, .alpha...	222	C15H26O	023178-88-3	53		
4	Lanosterol	426	C30H50O	000079-63-0	49		
5	2-Isopropenyl-4a,8-dimethyl-1,2...	204	C15H24	207297-57-2	42		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062338.D
Acq On : 8 Aug 2024 20:56
Operator : MA/JU
Sample : P3434-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E05T4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.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...	3.681	2.9	ng/ul	59446	1	7.957	411987	20.0
1-Phenoxypropan...	11.482	3.4	ng/ul	117445	2	10.748	683948	20.0
n-Hexadecanoic ...	18.214	6.3	ng/ul	404659	4	17.309	1275680	20.0
Pentafluoroprop...	21.227	2.9	ng/ul	214163	5	21.551	1457520	20.0
1,1,4a-Trimethy...	28.688	12.8	ng/ul	990303	6	24.635	1545570	20.0
9,19-Cyclolanos...	29.134	15.6	ng/ul	1206810	6	24.635	1545570	20.0