

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120221\
 Data File : VU046047.D
 Acq On : 02 Dec 2021 13:13
 Operator : SY/MD
 Sample : M4868-10ME
 Misc : 8.68g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGKP5ME

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\SFAMULM112921WMA.M
 Title : VOC Analysis

Signal : TIC: VU046047.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	72	80	101	rVB	79594	110184	7.84%	1.132%
2	1.915	170	179	198	rBV	47812	83107	5.91%	0.854%
3	1.989	198	202	209	rVV6	1227	1683	0.12%	0.017%
4	2.542	362	374	387	rBV	150862	246803	17.55%	2.536%
5	3.034	520	527	536	rVB5	1613	3094	0.22%	0.032%
6	3.112	547	551	554	rBV2	357	343	0.02%	0.004%
7	3.176	560	571	593	rVV2	7599	19862	1.41%	0.204%
8	4.655	1015	1031	1086	rBV2	42474	190790	13.57%	1.961%
9	4.976	1127	1131	1134	rBV2	323	300	0.02%	0.003%
10	5.063	1140	1158	1187	rVB	122926	304878	21.68%	3.133%
11	5.722	1343	1363	1388	rBV2	308110	786601	55.94%	8.083%
12	5.980	1431	1443	1459	rBV4	4151	10653	0.76%	0.109%
13	6.250	1512	1527	1559	rBV	243025	501951	35.70%	5.158%
14	6.539	1605	1617	1629	rBV5	13448	28969	2.06%	0.298%
15	6.600	1632	1636	1650	rVV6	2136	4284	0.30%	0.044%
16	6.693	1650	1665	1689	rVB	169428	350095	24.90%	3.598%
17	6.806	1696	1700	1707	rBB2	341	542	0.04%	0.006%
18	6.989	1754	1757	1764	rBV	158	264	0.02%	0.003%
19	7.189	1809	1819	1828	rBV4	1468	2661	0.19%	0.027%
20	7.237	1832	1834	1838	rVB3	528	398	0.03%	0.004%
21	7.568	1924	1937	1959	rVV	89584	176106	12.52%	1.810%
22	7.687	1970	1974	1982	rBV3	801	1102	0.08%	0.011%
23	7.796	1997	2008	2015	rBV4	1055	2195	0.16%	0.023%
24	7.899	2025	2040	2056	rBV	339991	644429	45.83%	6.622%
25	8.182	2116	2128	2152	rVV	56917	118388	8.42%	1.217%
26	8.549	2236	2242	2249	rVB4	1292	1847	0.13%	0.019%
27	8.677	2259	2282	2311	rBV2	121883	381859	27.16%	3.924%
28	8.954	2360	2368	2378	rBV2	563	1148	0.08%	0.012%
29	9.214	2441	2449	2460	rBV5	1512	1765	0.13%	0.018%
30	9.336	2481	2487	2494	rVB3	963	1045	0.07%	0.011%
31	9.423	2499	2514	2538	rVB	290892	636739	45.29%	6.543%
32	9.578	2549	2562	2576	rVB	8223	14808	1.05%	0.152%
33	9.700	2588	2600	2610	rBV2	33426	64284	4.57%	0.661%
34	9.806	2626	2633	2640	rVB	1178	1550	0.11%	0.016%
35	10.021	2692	2700	2711	rVB6	1351	2468	0.18%	0.025%
36	10.115	2715	2729	2742	rVV6	12023	25951	1.85%	0.267%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
 Title : VOC Analysis

37	10.166	2742	2745	2752	rVB2	830	970	0.07%	0.010%
38	10.253	2763	2772	2783	rVV5	3480	5823	0.41%	0.060%
39	10.311	2784	2790	2794	rVV3	555	625	0.04%	0.006%
40	10.356	2797	2804	2811	rVV6	2684	4388	0.31%	0.045%
41	10.394	2811	2816	2826	rVB3	1793	2767	0.20%	0.028%
42	10.468	2832	2839	2840	rBV3	683	522	0.04%	0.005%
43	10.491	2840	2846	2857	rVB2	3587	5970	0.42%	0.061%
44	10.558	2857	2867	2875	rBV2	2650	4486	0.32%	0.046%
45	10.626	2875	2888	2891	rBV6	2820	4627	0.33%	0.048%
46	10.725	2915	2919	2920	rBV2	618	487	0.03%	0.005%
47	10.770	2920	2933	2958	rVV	226230	393319	27.97%	4.042%
48	10.870	2959	2964	2965	rVV2	685	584	0.04%	0.006%
49	10.915	2968	2978	2984	rVB2	2842	4961	0.35%	0.051%
50	11.005	2997	3006	3019	rBV	11928	24362	1.73%	0.250%
51	11.114	3028	3040	3057	rVB3	28029	54641	3.89%	0.561%
52	11.205	3061	3068	3075	rBV6	1098	1510	0.11%	0.016%
53	11.246	3079	3081	3086	rVB5	613	419	0.03%	0.004%
54	11.304	3088	3099	3110	rBV7	6483	13972	0.99%	0.144%
55	11.417	3127	3134	3141	rVV4	8038	10607	0.75%	0.109%
56	11.475	3141	3152	3168	rVB	31561	56644	4.03%	0.582%
57	11.571	3176	3182	3191	rBV5	3377	6362	0.45%	0.065%
58	11.642	3199	3204	3214	rVB7	3174	4665	0.33%	0.048%
59	11.709	3214	3225	3232	rBV8	6350	12501	0.89%	0.128%
60	11.819	3247	3259	3271	rBV	408650	655989	46.65%	6.741%
61	11.877	3272	3277	3279	rBV4	3100	3426	0.24%	0.035%
62	12.102	3335	3347	3351	rBV4	6739	11601	0.83%	0.119%
63	12.198	3365	3377	3392	rVB	377548	623935	44.38%	6.412%
64	12.330	3408	3418	3428	rBV	34349	50624	3.60%	0.520%
65	12.385	3429	3435	3449	rVB	4938	10540	0.75%	0.108%
66	12.478	3455	3464	3465	rBV3	3739	5124	0.36%	0.053%
67	12.934	3598	3606	3611	rBV9	3644	6034	0.43%	0.062%
68	13.034	3630	3637	3649	rVB6	8718	17779	1.26%	0.183%
69	13.288	3710	3716	3718	rBV5	2189	2204	0.16%	0.023%
70	13.352	3729	3736	3744	rBV7	2404	3904	0.28%	0.040%
71	13.433	3753	3761	3765	rBV	13692	19320	1.37%	0.199%
72	13.629	3817	3822	3835	rVB	2896	4770	0.34%	0.049%
73	13.841	3881	3888	3893	rBV8	3957	5866	0.42%	0.060%
74	13.947	3915	3921	3923	rBV4	1369	1496	0.11%	0.015%
75	14.028	3943	3946	3947	rBV3	1058	547	0.04%	0.006%
76	14.089	3953	3965	3981	rVB	356741	556050	39.55%	5.714%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

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Filtering: 5

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 Title : VOC Analysis

77	14.339	4039	4043	4052	rVB7	1549	2268	0.16%	0.023%
78	14.384	4054	4057	4059	rBV4	820	563	0.04%	0.006%
79	14.452	4072	4078	4084	rVB2	8640	9911	0.70%	0.102%
80	14.783	4177	4181	4183	rBV4	945	763	0.05%	0.008%
81	14.809	4184	4189	4196	rVV6	2722	4011	0.29%	0.041%
82	14.880	4206	4211	4220	rVB4	4689	6256	0.44%	0.064%
83	14.944	4224	4231	4236	rBV9	1522	2736	0.19%	0.028%
84	15.024	4248	4256	4263	rBV9	3028	5493	0.39%	0.056%
85	15.169	4297	4301	4306	rBV	5972	6665	0.47%	0.068%
86	15.224	4307	4318	4340	rVB	894229	1406044	100.00%	14.449%
87	15.339	4347	4354	4364	rBV	9465	13938	0.99%	0.143%
88	15.410	4364	4376	4400	rVB	357866	580594	41.29%	5.966%
89	15.593	4429	4433	4434	rBV3	889	685	0.05%	0.007%
90	15.741	4476	4479	4482	rBV4	644	527	0.04%	0.005%
91	15.767	4482	4487	4492	rVB8	1044	1141	0.08%	0.012%
92	15.902	4527	4529	4530	rBV3	1000	443	0.03%	0.005%
93	15.954	4534	4545	4559	rVB	71452	115170	8.19%	1.183%
94	16.146	4597	4605	4613	rBV	22054	32521	2.31%	0.334%
95	16.262	4631	4641	4660	rVB2	43398	85216	6.06%	0.876%
96	16.407	4676	4686	4693	rBV2	42228	67242	4.78%	0.691%
97	16.445	4694	4698	4712	rVB	24655	33932	2.41%	0.349%
98	16.831	4816	4818	4825	rBV5	822	839	0.06%	0.009%
99	16.880	4827	4833	4842	rVB4	7399	10535	0.75%	0.108%
100	17.098	4893	4901	4909	rBV3	15550	26293	1.87%	0.270%

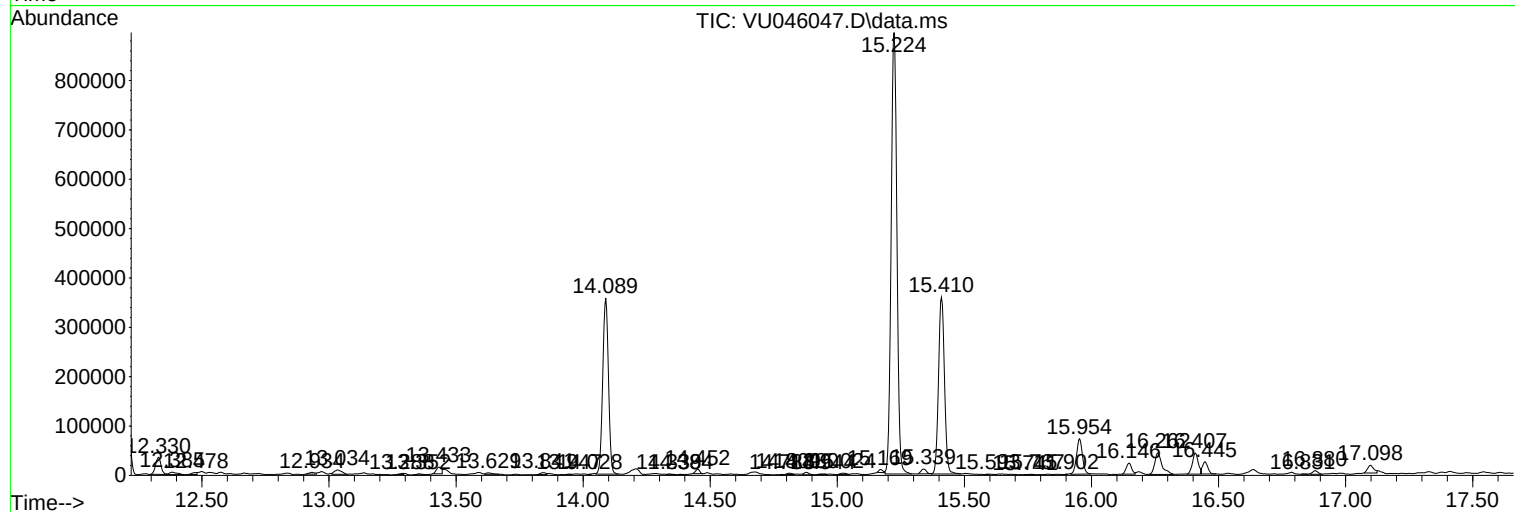
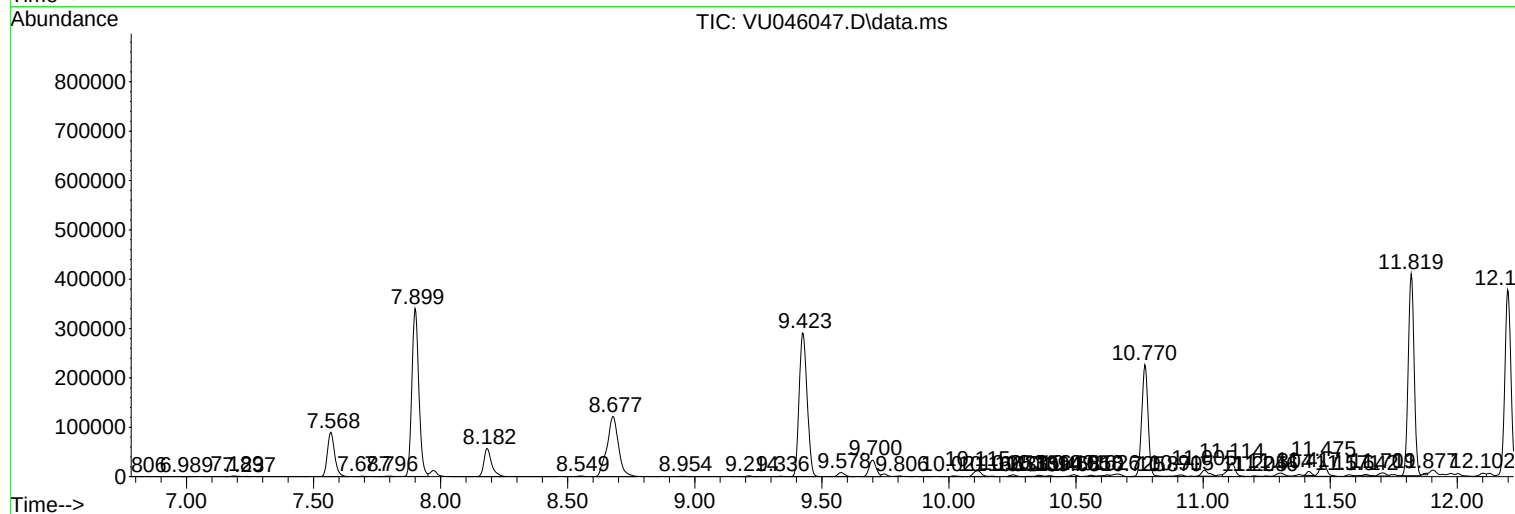
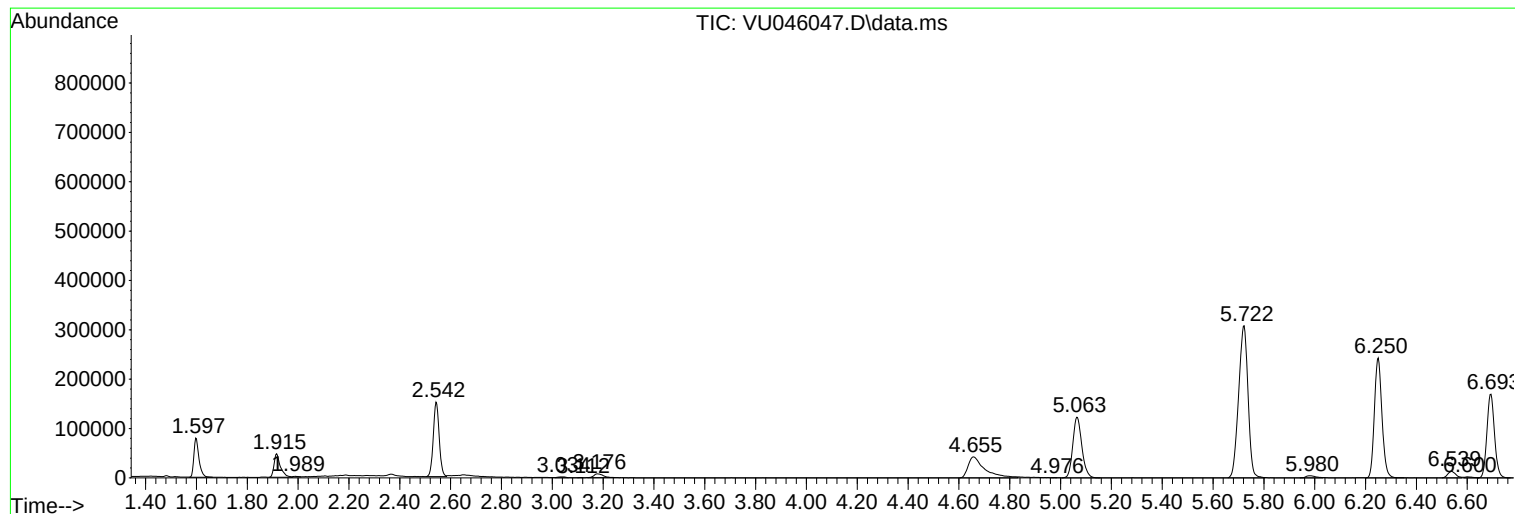
Sum of corrected areas: 9731353

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Instrument :
MSVOA_U
ClientSampleId :
BGKP5ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_U
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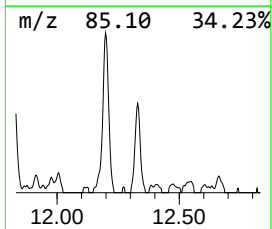
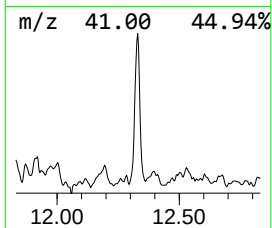
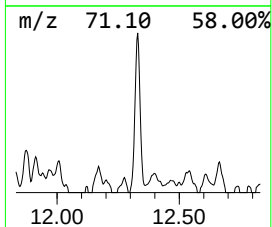
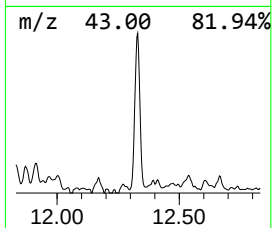
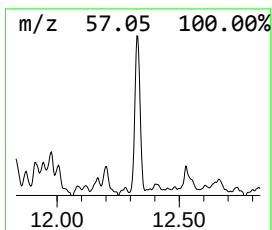
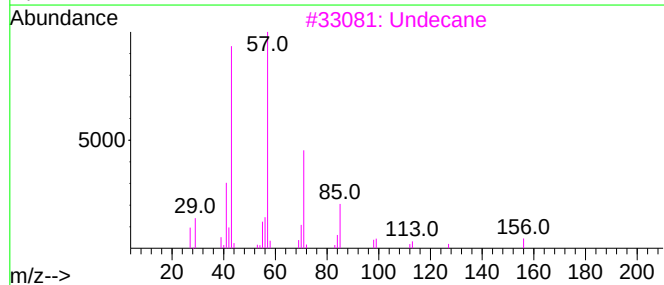
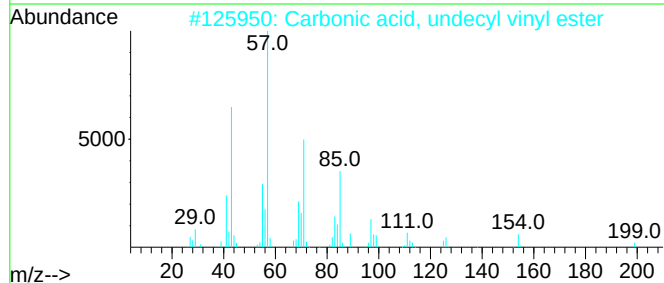
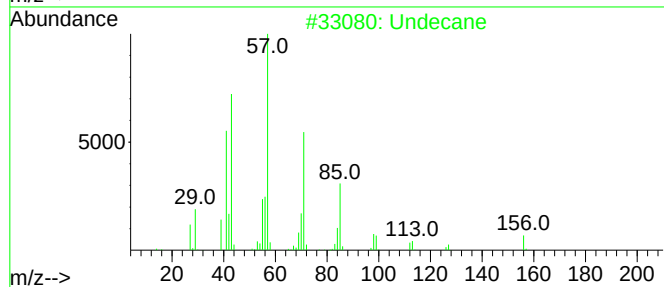
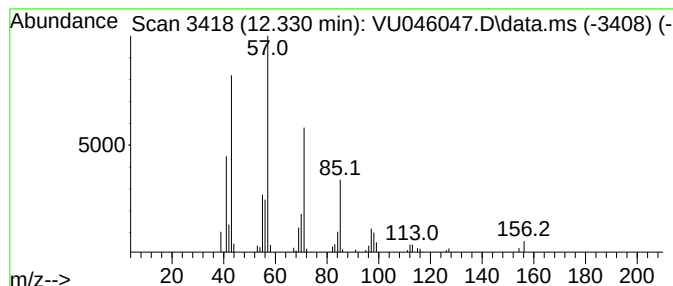
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.330	3.86 ug/L	50624	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane	156	C11H24	001120-21-4	96
2			Carbonic acid, undecyl vinyl ester	242	C14H26O3	1000382-54-9	83
3			Undecane	156	C11H24	001120-21-4	81
4			Undecane	156	C11H24	001120-21-4	81
5			Undecane	156	C11H24	001120-21-4	76



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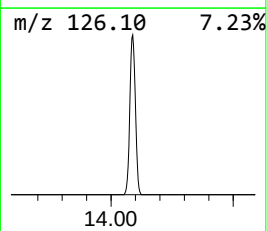
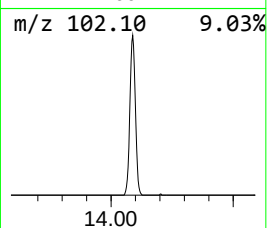
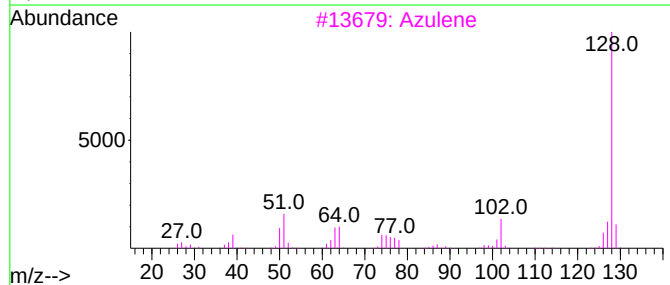
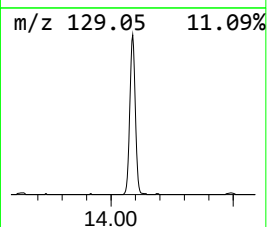
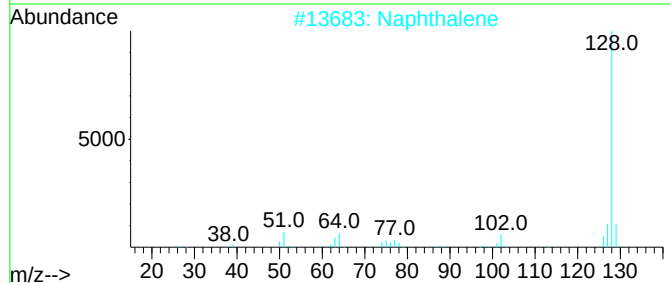
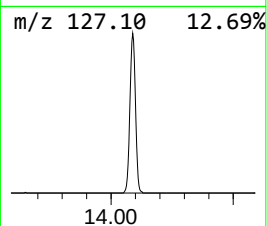
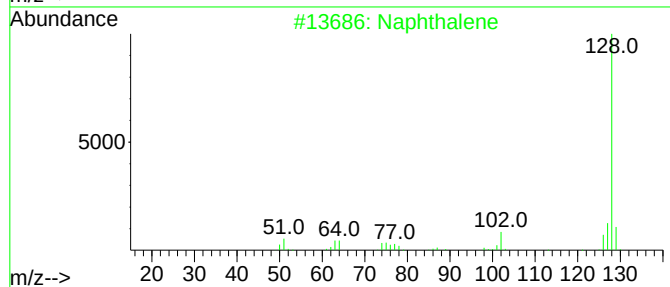
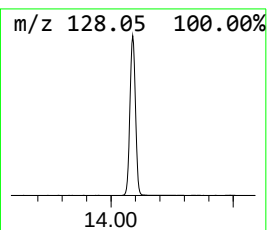
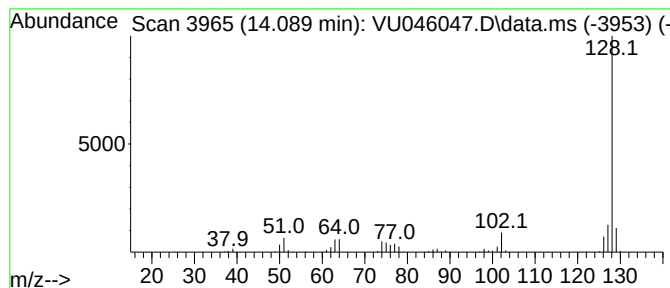
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Azulene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.089	42.38 ug/L	556050	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Naphthalene	128	C10H8	000091-20-3	95
3			Azulene	128	C10H8	000275-51-4	91
4			Azulene	128	C10H8	000275-51-4	91
5			Naphthalene	128	C10H8	000091-20-3	91



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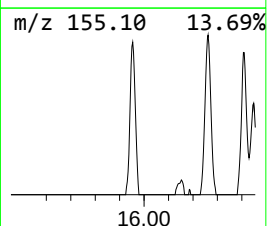
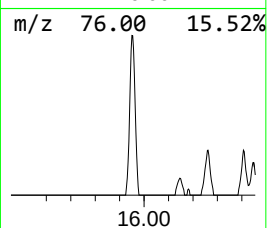
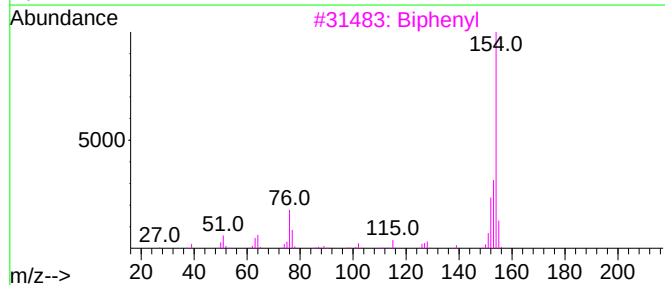
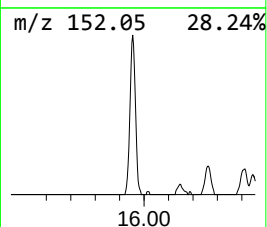
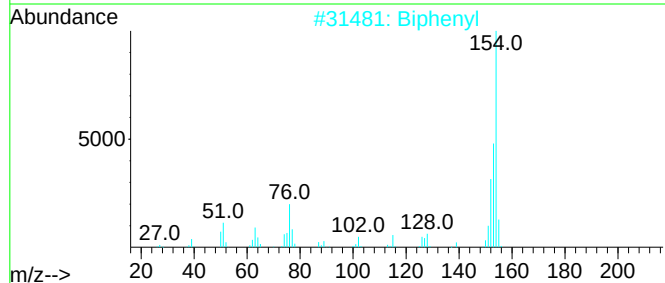
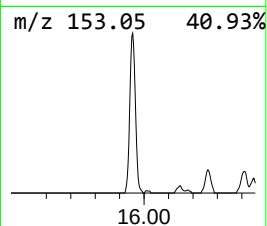
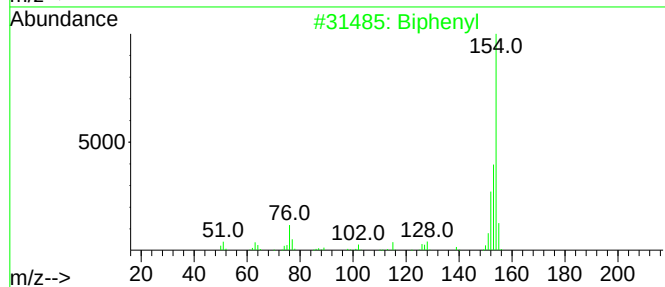
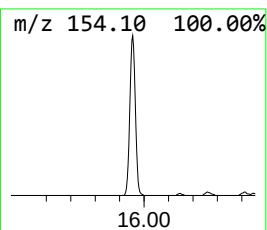
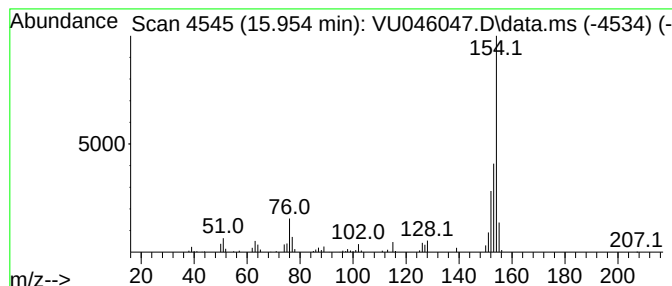
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Quant Title : VOC Analysis

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

Peak Number 7 Naphthalene, 2-ethenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.954	8.78 ug/L	115170	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Biphenyl	154	C12H10	000092-52-4	95
2			Biphenyl	154	C12H10	000092-52-4	93
3			Biphenyl	154	C12H10	000092-52-4	90
4			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	87
5			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120221\
Data File : VU046047.D
Acq On : 02 Dec 2021 13:13
Operator : SY/MD
Sample : M4868-10ME
Misc : 8.68g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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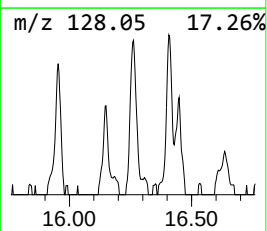
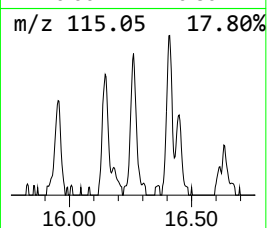
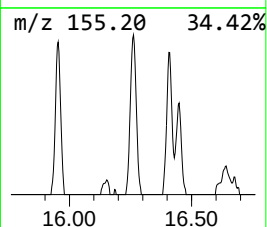
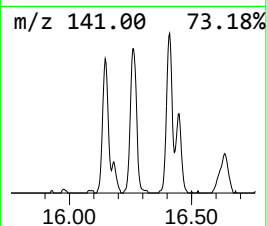
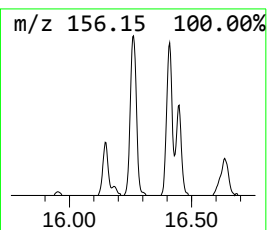
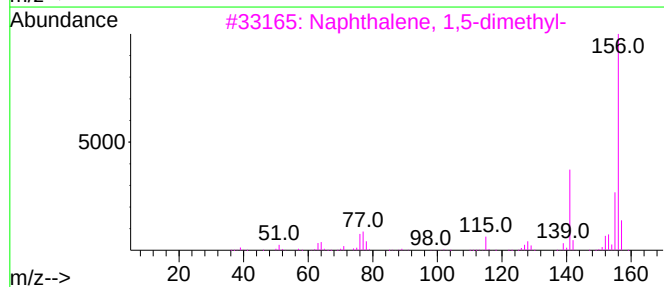
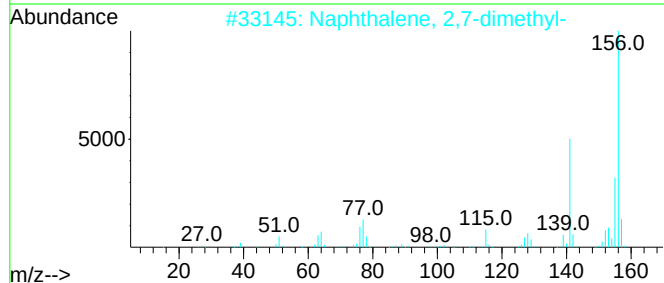
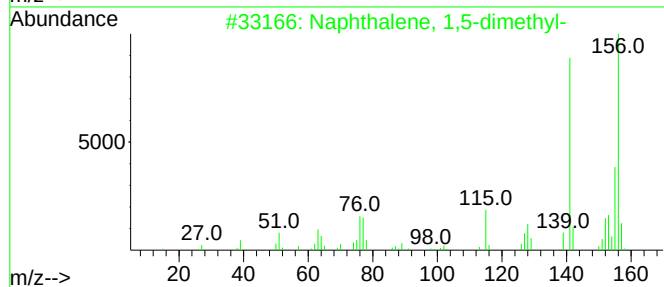
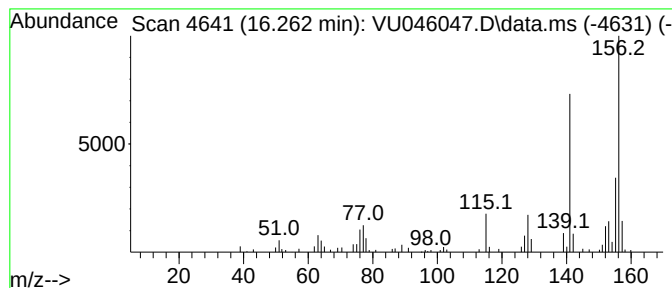
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Quant Title : VOC Analysis

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

Peak Number 8 Naphthalene, 1,5-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.262	6.50 ug/L	85216	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	98
2			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
3			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97
4			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
5			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120221\
Data File : VU046047.D
Acq On : 02 Dec 2021 13:13
Operator : SY/MD
Sample : M4868-10ME
Misc : 8.68g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGKP5ME

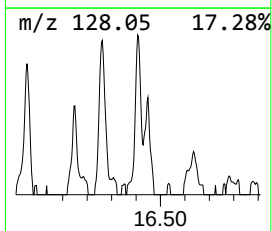
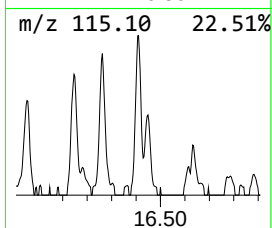
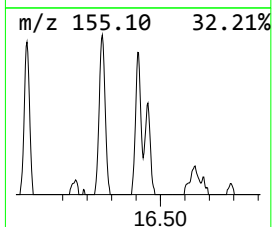
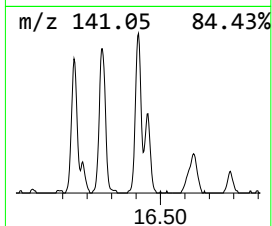
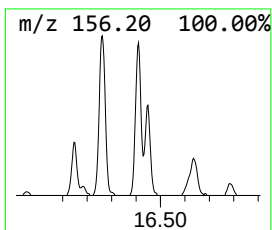
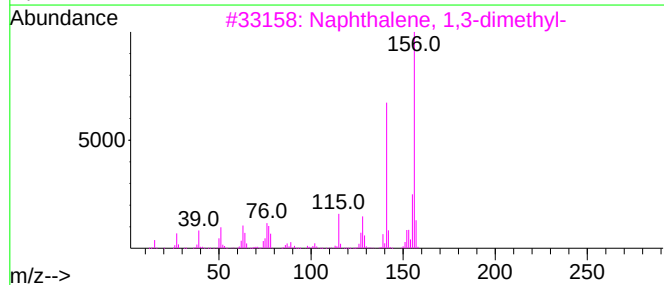
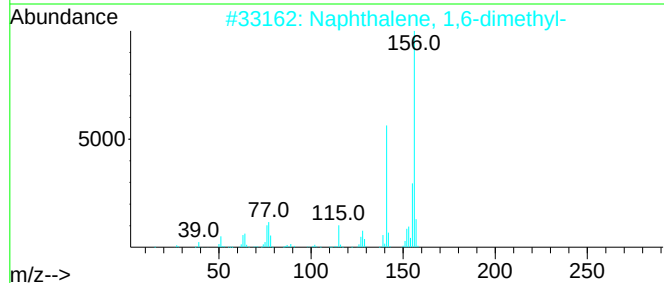
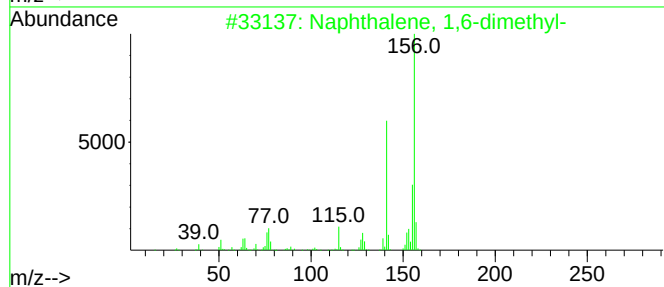
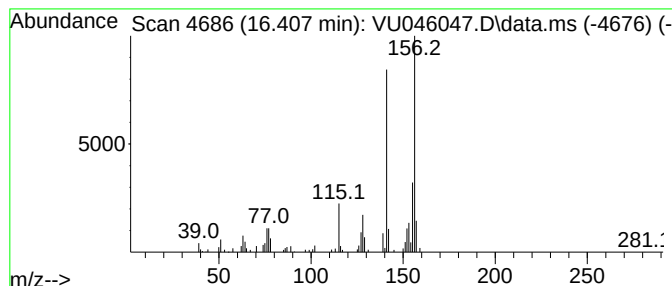
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Quant Title : VOC Analysis

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

Peak Number 9 Naphthalene, 1,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.407	5.13 ug/L	67242	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
2			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
3			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
4			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
5			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120221\
Data File : VU046047.D
Acq On : 02 Dec 2021 13:13
Operator : SY/MD
Sample : M4868-10ME
Misc : 8.68g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGKP5ME

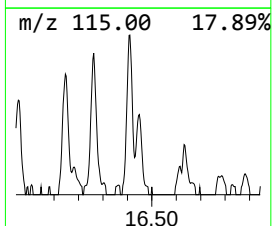
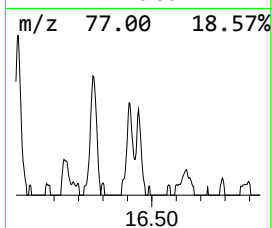
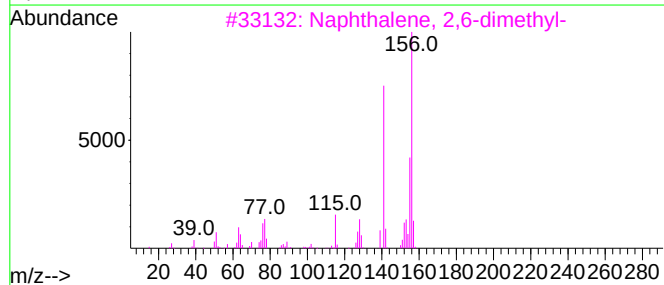
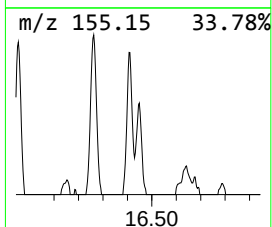
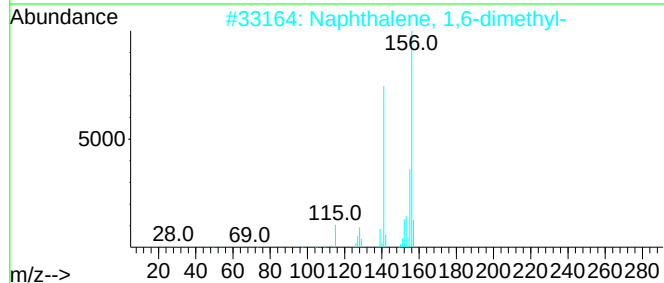
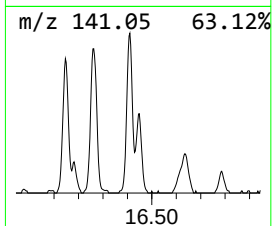
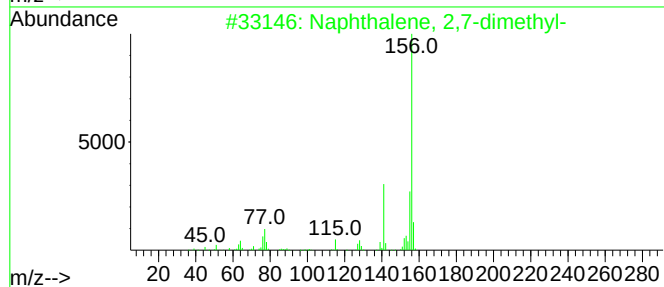
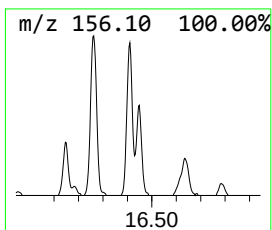
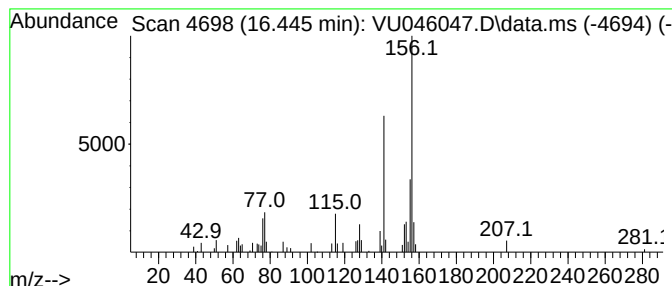
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Quant Title : VOC Analysis

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

Peak Number 10 Naphthalene, 2,7-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.445	2.59 ug/L	33932	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
2			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	95
3			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	95
4			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	94
5			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120221\
Data File : VU046047.D
Acq On : 02 Dec 2021 13:13
Operator : SY/MD
Sample : M4868-10ME
Misc : 8.68g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGKP5ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.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
(DEL) Alkane: S...	12.330	3.9	ug/L	50624	3	11.819	655989	50.0
Azulene	14.089	42.4	ug/L	556050	3	11.819	655989	50.0
Naphthalene, 2-...	15.954	8.8	ug/L	115170	3	11.819	655989	50.0
Naphthalene, 1,...	16.262	6.5	ug/L	85216	3	11.819	655989	50.0
Naphthalene, 1,...	16.407	5.1	ug/L	67242	3	11.819	655989	50.0
Naphthalene, 2,...	16.445	2.6	ug/L	33932	3	11.819	655989	50.0