

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042022\
 Data File : VU048154.D
 Acq On : 20 Apr 2022 19:37
 Operator : SY/MD
 Sample : N2485-15
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0J22

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\SFAMULM032422WMA.M
 Title : VOC Analysis

Signal : TIC: VU048154.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.359	3	6	22	rVB2	72657	72204	0.01%	0.003%
2	1.501	41	50	51	rBV6	8400	10856	0.00%	0.000%
3	1.597	71	80	93	rBV	158912	210003	0.03%	0.008%
4	1.732	118	122	129	rVB	9279	9313	0.00%	0.000%
5	1.913	169	178	196	rVV	117443	168844	0.02%	0.007%
6	1.993	199	203	215	rVB2	8002	11405	0.00%	0.000%
7	2.157	247	254	262	rVV3	8409	12049	0.00%	0.000%
8	2.205	263	269	281	rVB4	5443	8874	0.00%	0.000%
9	2.321	297	305	314	rBV4	5081	7813	0.00%	0.000%
10	2.414	327	334	346	rVB6	7962	14229	0.00%	0.001%
11	2.568	366	382	391	rBV	256762	424082	0.05%	0.017%
12	2.630	391	401	414	rVV	474396	867689	0.11%	0.034%
13	2.687	414	419	430	rVV	38396	65096	0.01%	0.003%
14	2.774	430	446	499	rVV	1739183	5052137	0.62%	0.200%
15	3.048	517	531	548	rBV	316207	653288	0.08%	0.026%
16	3.138	549	559	585	rVB	136833	287577	0.04%	0.011%
17	3.253	593	595	602	rVB5	722	691	0.00%	0.000%
18	3.363	620	629	642	rVB7	2919	6740	0.00%	0.000%
19	3.440	651	653	661	rVB5	594	703	0.00%	0.000%
20	3.581	692	697	699	rBV4	1368	1247	0.00%	0.000%
21	3.703	725	735	744	rVB6	1410	3168	0.00%	0.000%
22	3.787	753	761	771	rBV8	2575	4446	0.00%	0.000%
23	3.867	778	786	797	rBV3	2455	4475	0.00%	0.000%
24	3.925	800	804	811	rVB5	844	1031	0.00%	0.000%
25	4.044	835	841	843	rBV4	691	571	0.00%	0.000%
26	4.462	963	971	975	rBV6	517	749	0.00%	0.000%
27	4.536	975	994	1011	rBV	151118	382815	0.05%	0.015%
28	4.626	1011	1022	1039	rVV	132908	328713	0.04%	0.013%
29	4.710	1040	1048	1071	rVB	33899	84231	0.01%	0.003%
30	4.826	1082	1084	1091	rVB4	551	499	0.00%	0.000%
31	5.089	1141	1166	1196	rBV2	1971525	4718094	0.58%	0.187%
32	5.260	1217	1219	1224	rVV3	549	503	0.00%	0.000%
33	5.295	1224	1230	1239	rVB5	1445	2219	0.00%	0.000%
34	5.395	1244	1261	1279	rBV2	89809	211626	0.03%	0.008%
35	5.533	1288	1304	1322	rVB2	72124	167657	0.02%	0.007%
36	5.642	1334	1338	1345	rVB4	1502	1626	0.00%	0.000%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
 Title : VOC Analysis

37	5.845	1345	1401	1417	rBV5	111024998	543177923	66.88%	21.546%
38	5.938	1420	1430	1488	rVB	1714345	4776946	0.59%	0.189%
39	6.253	1518	1528	1553	rVB	497186	973777	0.12%	0.039%
40	6.549	1603	1620	1632	rVB10	10528	25453	0.00%	0.001%
41	6.694	1651	1665	1681	rBV	297660	599384	0.07%	0.024%
42	6.858	1709	1716	1729	rVB10	3229	5126	0.00%	0.000%
43	6.935	1736	1740	1745	rVB6	1013	999	0.00%	0.000%
44	6.983	1749	1755	1765	rVB7	2774	3918	0.00%	0.000%
45	7.073	1779	1783	1789	rBV4	677	750	0.00%	0.000%
46	7.108	1789	1794	1801	rVV5	1522	1780	0.00%	0.000%
47	7.153	1804	1808	1809	rVV2	836	607	0.00%	0.000%
48	7.186	1809	1818	1833	rVB6	4607	9676	0.00%	0.000%
49	7.411	1878	1888	1898	rVB8	3377	6328	0.00%	0.000%
50	7.465	1903	1905	1908	rBV4	672	480	0.00%	0.000%
51	7.568	1921	1937	1951	rBV	154762	274725	0.03%	0.011%
52	7.639	1956	1959	1967	rVB7	1240	1363	0.00%	0.000%
53	7.694	1968	1976	1991	rVB6	4228	8801	0.00%	0.000%
54	7.800	1998	2009	2026	rBV5	8912	20025	0.00%	0.001%
55	7.903	2026	2041	2054	rBV	581598	1074587	0.13%	0.043%
56	7.977	2054	2064	2076	rVB	122646	225606	0.03%	0.009%
57	8.182	2116	2128	2146	rBV	107784	195747	0.02%	0.008%
58	8.407	2188	2198	2202	rBV8	2693	4253	0.00%	0.000%
59	8.481	2218	2221	2222	rBV2	993	523	0.00%	0.000%
60	8.491	2222	2224	2235	rVB6	1739	2632	0.00%	0.000%
61	8.559	2235	2245	2258	rBV5	11734	22787	0.00%	0.001%
62	8.642	2258	2271	2308	rBV	255864	845858	0.10%	0.034%
63	8.948	2354	2366	2367	rBV8	1240	1970	0.00%	0.000%
64	9.176	2433	2437	2442	rVB4	592	622	0.00%	0.000%
65	9.366	2491	2496	2499	rBV2	527	510	0.00%	0.000%
66	9.513	2499	2542	2559	rBV2	119125110	812206846	100.00%	32.218%
67	10.115	2722	2729	2731	rBV4	6862	8131	0.00%	0.000%
68	10.603	2876	2881	2894	rVB4	6362	9888	0.00%	0.000%
69	10.677	2898	2904	2914	rVB7	3620	5858	0.00%	0.000%
70	10.764	2918	2931	2936	rBV	529392	926157	0.11%	0.037%
71	10.896	2970	2972	2973	rBV2	1433	656	0.00%	0.000%
72	10.996	2993	3003	3014	rVB	41327	67696	0.01%	0.003%
73	11.063	3017	3024	3028	rVV7	3514	4667	0.00%	0.000%
74	11.105	3029	3037	3050	rVB3	19818	33966	0.00%	0.001%
75	11.253	3075	3083	3091	rVB3	3921	6403	0.00%	0.000%
76	11.388	3121	3125	3128	rBV5	1470	1147	0.00%	0.000%

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 Title : VOC Analysis

77	11.472	3144	3151	3153	rBV4	2908	3239	0.00%	0.000%
78	11.661	3206	3210	3213	rVB6	771	599	0.00%	0.000%
79	11.764	3215	3242	3256	rBV	22831455	52526939	6.47%	2.084%
80	11.896	3256	3283	3323	rVB9	129733215	517302405	63.69%	20.520%
81	12.279	3368	3402	3454	rBV7	130511391	521763866	64.24%	20.697%
82	12.697	3525	3532	3543	rVB2	19173	28815	0.00%	0.001%
83	12.912	3593	3599	3607	rBV8	6258	9947	0.00%	0.000%
84	12.973	3608	3618	3638	rVB	309507	487627	0.06%	0.019%
85	13.095	3650	3656	3663	rVB4	7228	9724	0.00%	0.000%
86	13.166	3664	3678	3687	rBV6	27726	71278	0.01%	0.003%
87	13.330	3719	3729	3745	rVB	134598	219387	0.03%	0.009%
88	13.504	3777	3783	3793	rVB5	6166	10133	0.00%	0.000%
89	13.578	3799	3806	3815	rVB7	5443	9342	0.00%	0.000%
90	13.652	3822	3829	3839	rBV6	2840	4717	0.00%	0.000%
91	13.848	3873	3890	3913	rBV	25634471	39994831	4.92%	1.586%
92	14.089	3960	3965	3975	rVB3	4662	7286	0.00%	0.000%
93	14.330	4026	4040	4063	rBV	5688895	8962333	1.10%	0.356%
94	14.732	4158	4165	4175	rVB6	6450	10358	0.00%	0.000%
95	14.828	4187	4195	4203	rBV7	2908	5442	0.00%	0.000%
96	15.417	4364	4378	4392	rVB2	59209	101740	0.01%	0.004%
97	15.471	4392	4395	4398	rBV4	1046	837	0.00%	0.000%
98	15.507	4404	4406	4409	rBV4	1144	685	0.00%	0.000%
99	15.999	4548	4559	4574	rBV2	81591	135397	0.02%	0.005%
100	16.089	4585	4587	4590	rBV3	979	727	0.00%	0.000%

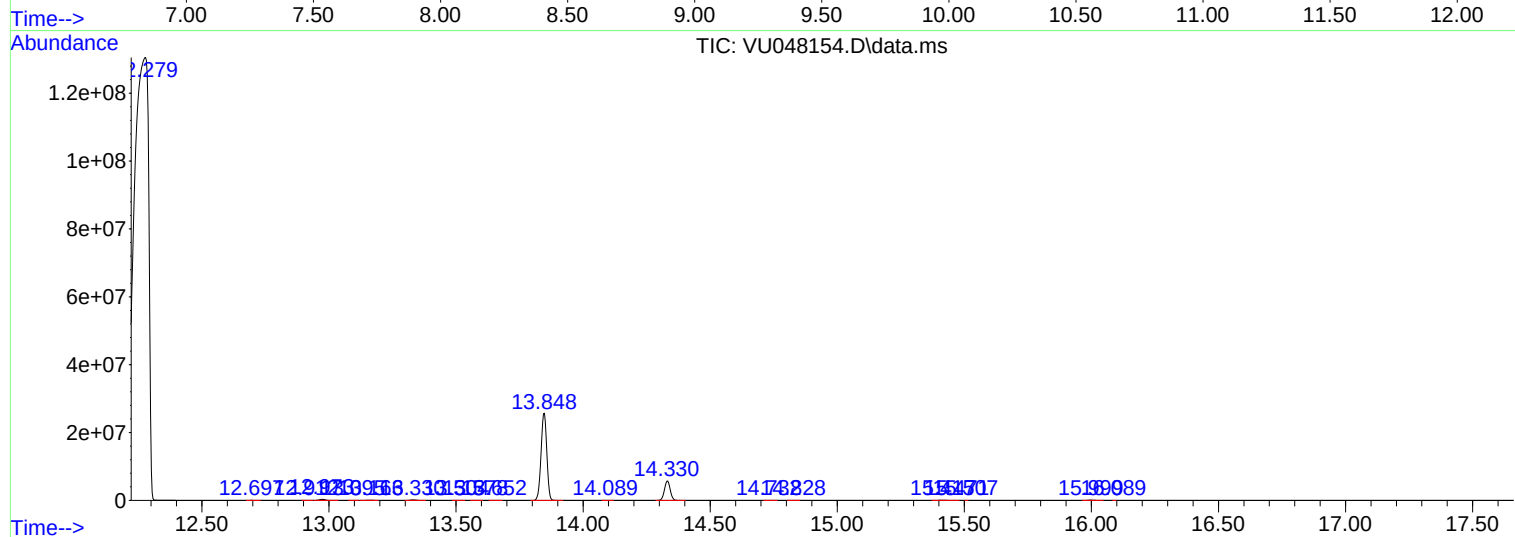
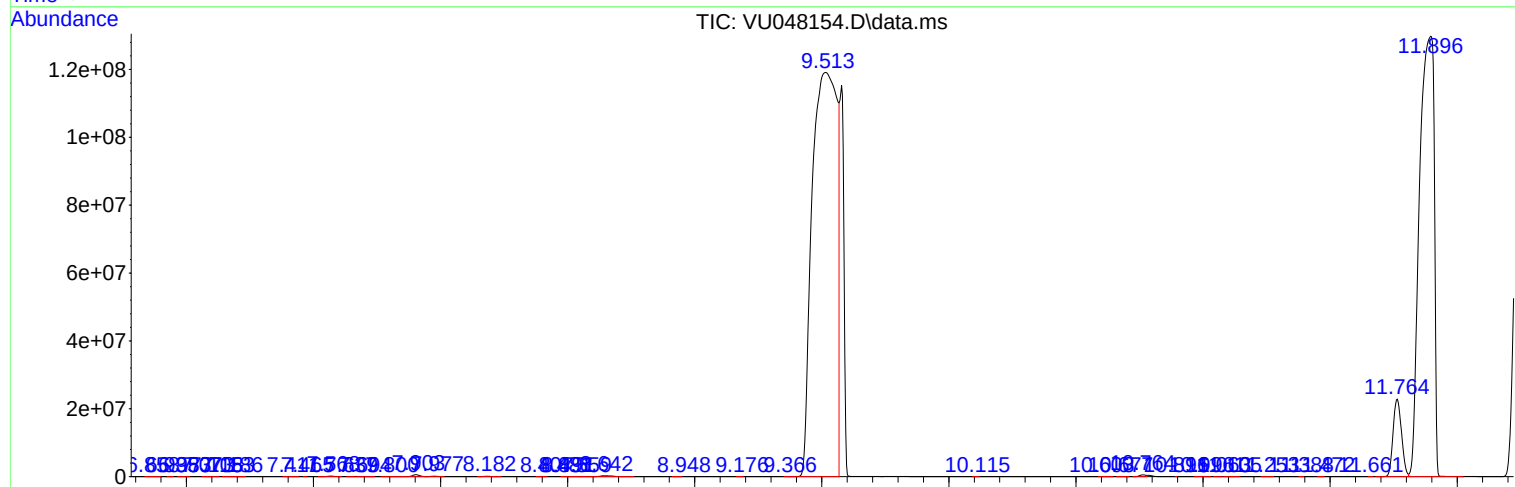
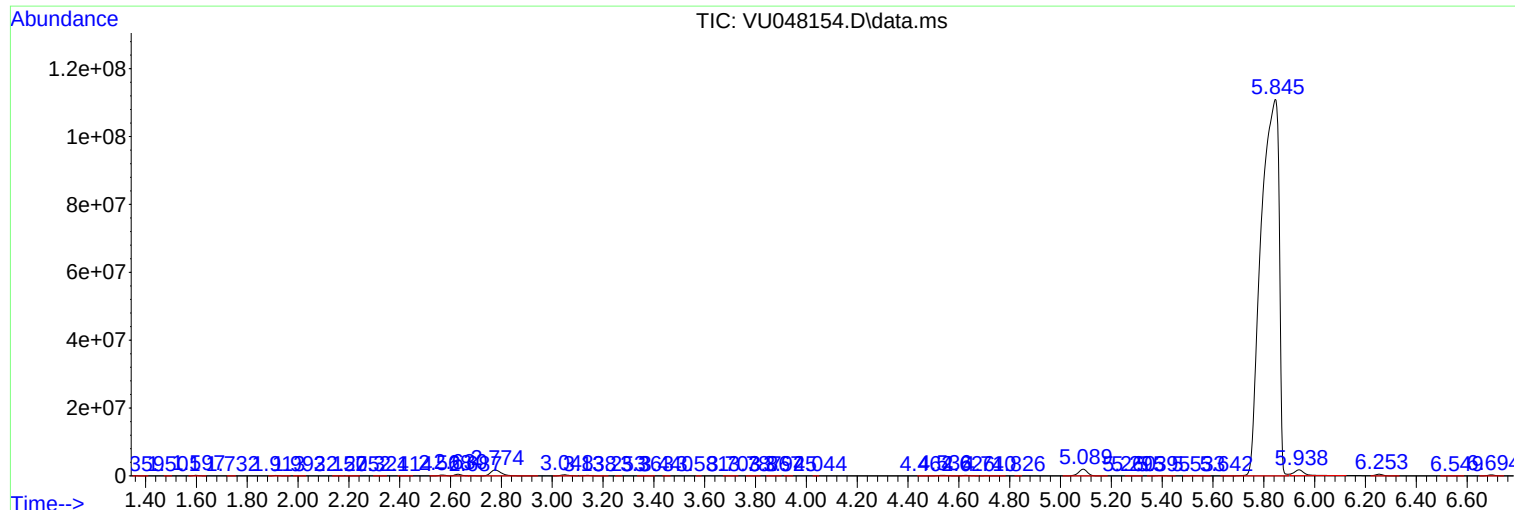
Sum of corrected areas: 2520999488

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ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
C0J22

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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



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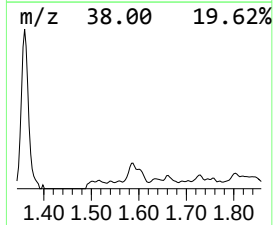
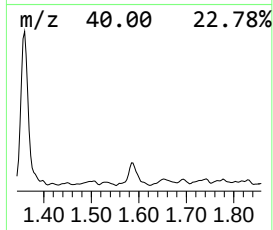
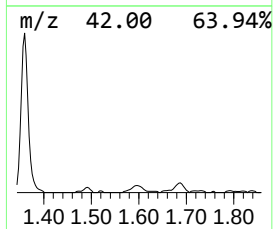
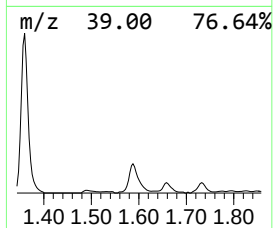
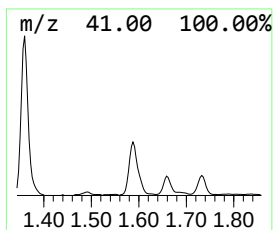
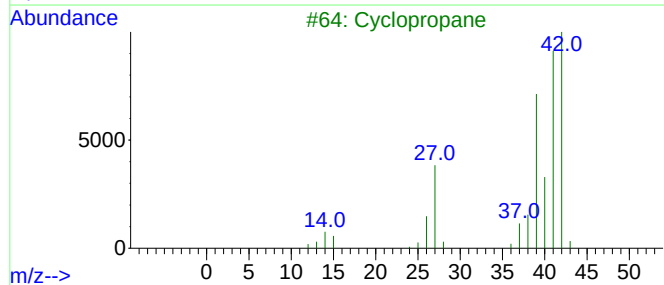
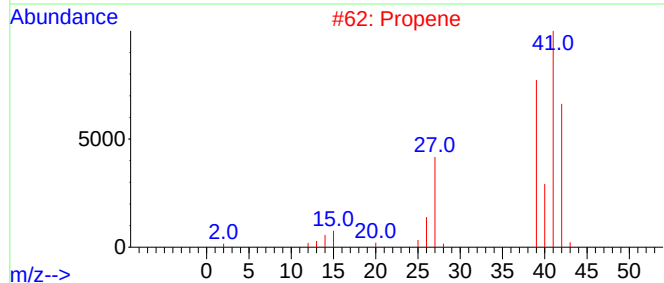
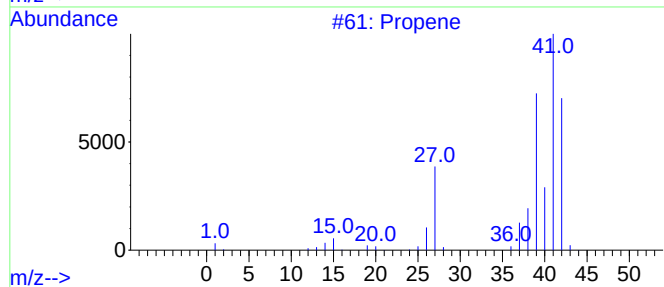
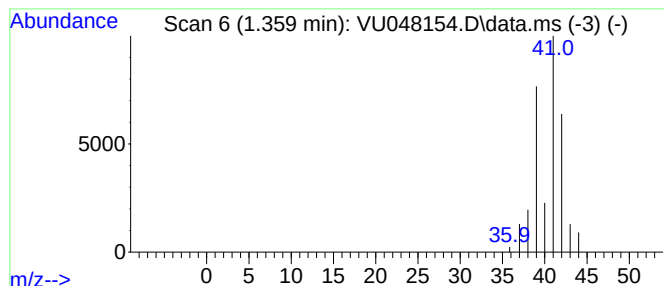
Instrument :
MSVOA_U
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.359	3.71 ug/L	72204	1,4-Difluorobenzene	6.253	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	90
2	Propene	42	C3H6	000115-07-1	45
3	Cyclopropane	42	C3H6	000075-19-4	9
4	Cyclopropene	40	C3H4	002781-85-3	9
5	Cyclopropane	42	C3H6	000075-19-4	7



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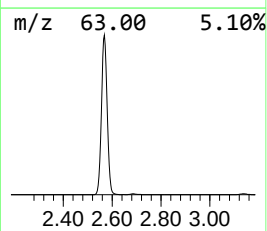
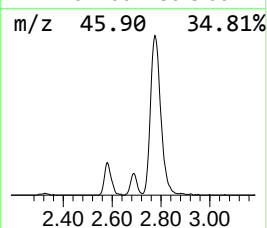
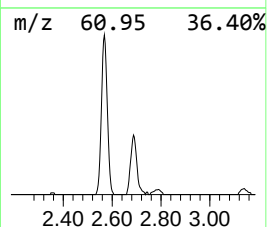
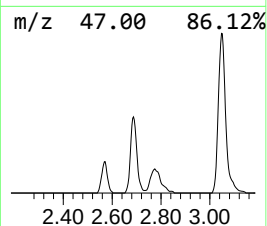
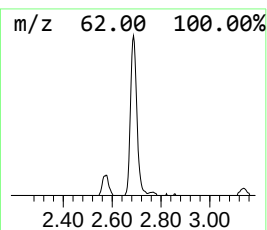
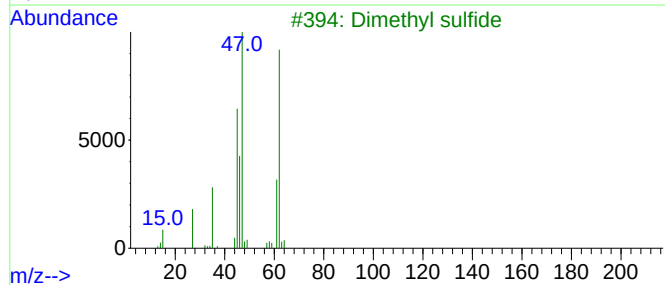
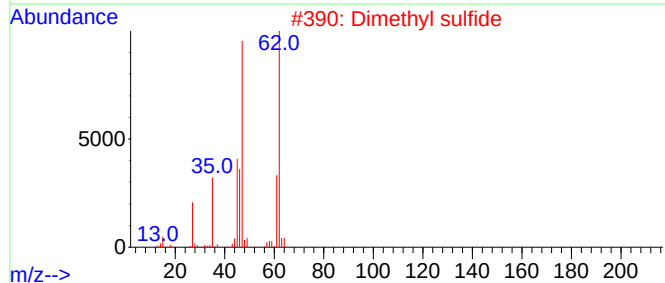
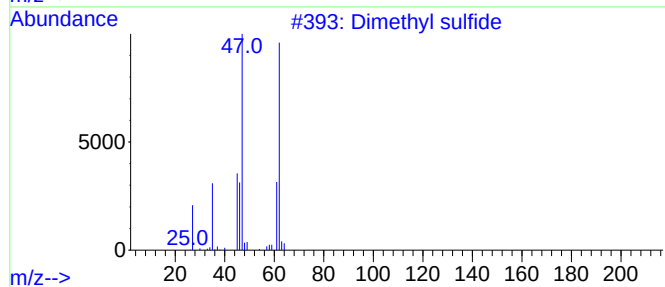
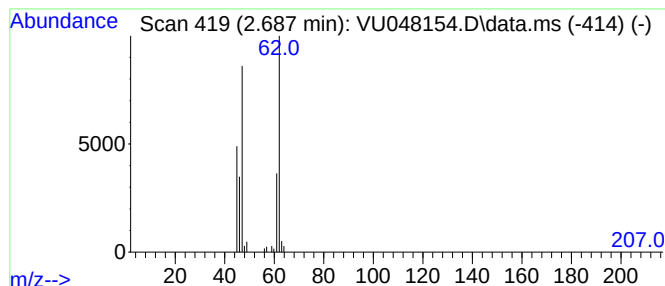
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Dimethyl sulfide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.687	3.34 ug/L	65096	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl sulfide	62	C2H6S	000075-18-3	91
2			Dimethyl sulfide	62	C2H6S	000075-18-3	91
3			Dimethyl sulfide	62	C2H6S	000075-18-3	91
4			Ethanethiol	62	C2H6S	000075-08-1	78
5			Ethanethiol	62	C2H6S	000075-08-1	72



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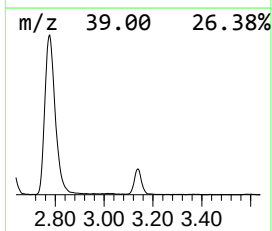
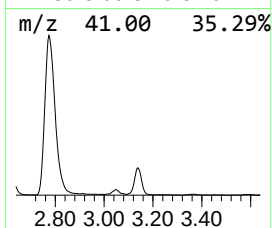
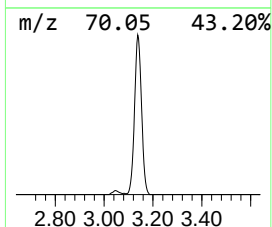
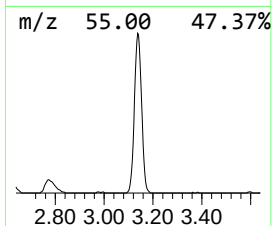
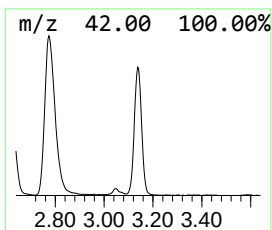
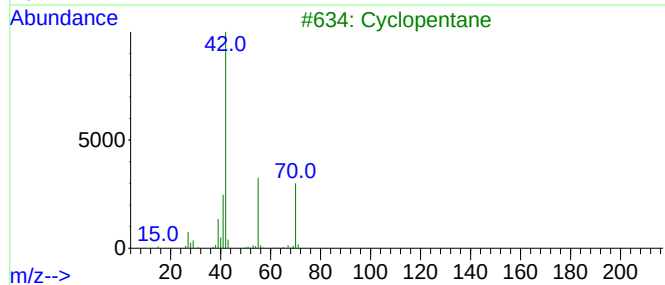
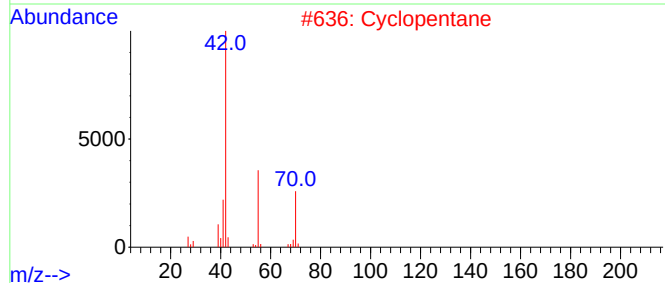
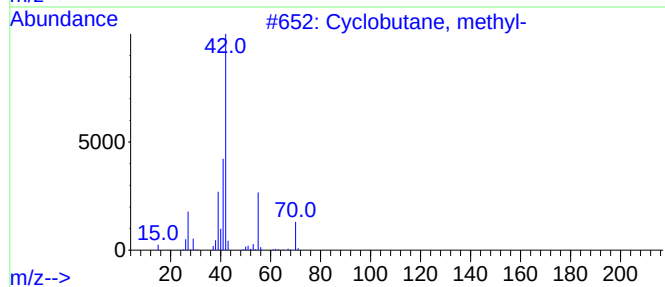
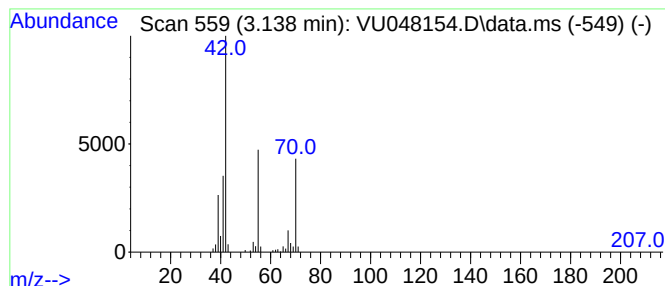
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Cyclic3.138 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.138	14.77 ug/L	287577	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclobutane, methyl-	70	C5H10	000598-61-8	80
2			Cyclopentane	70	C5H10	000287-92-3	80
3			Cyclopentane	70	C5H10	000287-92-3	72
4			1-Pentene	70	C5H10	000109-67-1	72
5			1-Pentene	70	C5H10	000109-67-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042022\
Data File : VU048154.D
Acq On : 20 Apr 2022 19:37
Operator : SY/MD
Sample : N2485-15
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0J22

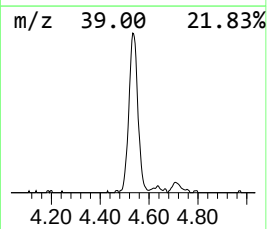
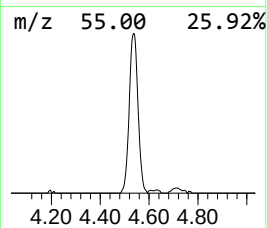
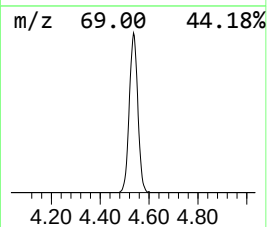
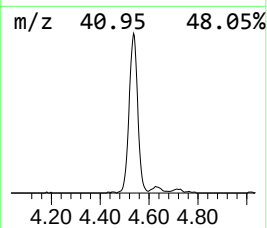
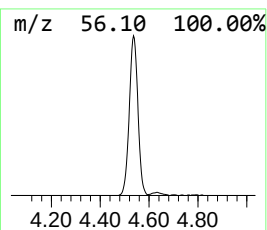
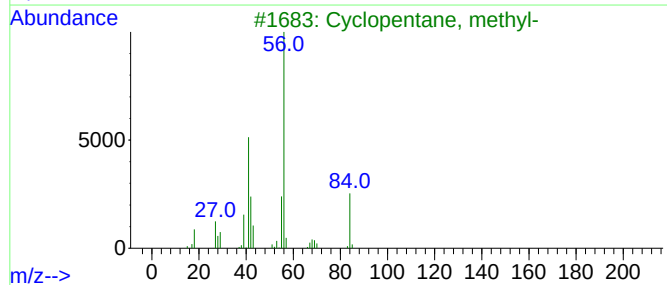
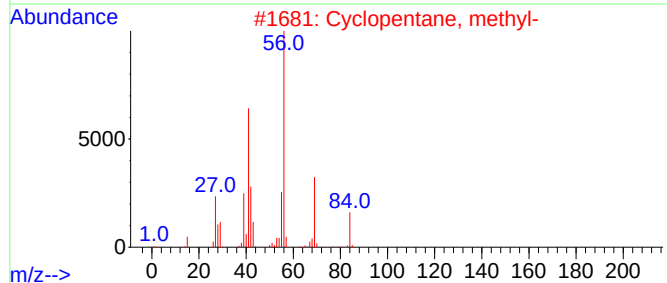
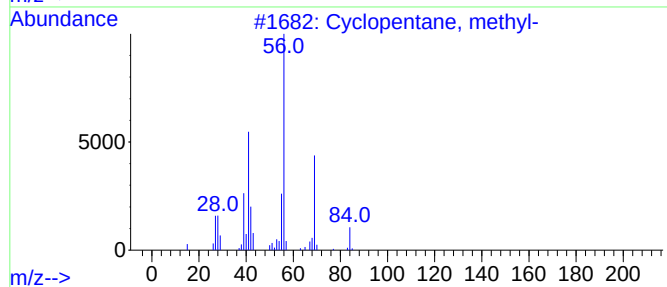
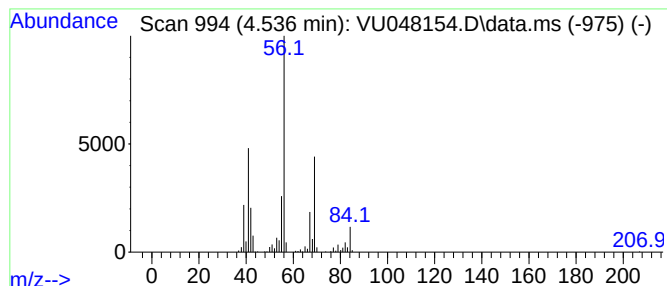
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Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Cyclic4.536 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.536	19.66 ug/L	382815	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	87
2			Cyclopentane, methyl-	84	C6H12	000096-37-7	74
3			Cyclopentane, methyl-	84	C6H12	000096-37-7	72
4			Cyclopentane, methyl-	84	C6H12	000096-37-7	72
5			Cyclohexane	84	C6H12	000110-82-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042022\
Data File : VU048154.D
Acq On : 20 Apr 2022 19:37
Operator : SY/MD
Sample : N2485-15
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0J22

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.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...	1.359	3.7	ug/L	72204	1	6.253	973777	50.0
Dimethyl sulfide	2.687	3.3	ug/L	65096	1	6.253	973777	50.0
(DEL) Alkane: C...	3.138	14.8	ug/L	287577	1	6.253	973777	50.0
(DEL) Alkane: C...	4.536	19.7	ug/L	382815	1	6.253	973777	50.0