

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120421\
 Data File : VU046097.D
 Acq On : 04 Dec 2021 16:43
 Operator : SY/MD
 Sample : M4942-09
 Misc : 6.84g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGKR1

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: VU046097.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	97	rBV	155895	203719	13.28%	1.763%
2	1.861	156	162	169	rBV2	1766	2337	0.15%	0.020%
3	1.916	170	179	199	rVV	95288	158569	10.34%	1.372%
4	2.546	363	375	390	rBV	301545	491123	32.02%	4.251%
5	2.986	510	512	516	rVB3	300	220	0.01%	0.002%
6	3.041	520	529	537	rVB4	1734	2904	0.19%	0.025%
7	3.092	541	545	551	rVB4	385	343	0.02%	0.003%
8	3.118	551	553	558	rBV2	215	119	0.01%	0.001%
9	3.179	558	572	592	rBV	12848	33212	2.17%	0.287%
10	3.369	628	631	640	rVB	384	481	0.03%	0.004%
11	3.436	649	652	658	rBV	153	216	0.01%	0.002%
12	3.620	705	709	712	rBV	170	184	0.01%	0.002%
13	4.028	833	836	839	rBB	142	121	0.01%	0.001%
14	4.182	881	884	886	rBV	153	128	0.01%	0.001%
15	4.652	1013	1030	1078	rBV	77180	338818	22.09%	2.933%
16	5.063	1141	1158	1186	rVB	248711	590273	38.48%	5.109%
17	5.182	1193	1195	1197	rBB	233	126	0.01%	0.001%
18	5.234	1206	1211	1214	rBB	144	147	0.01%	0.001%
19	5.269	1218	1222	1225	rBB	233	164	0.01%	0.001%
20	5.288	1225	1228	1229	rBV2	242	137	0.01%	0.001%
21	5.324	1236	1239	1243	rBV2	233	218	0.01%	0.002%
22	5.629	1330	1334	1338	rBV	146	187	0.01%	0.002%
23	5.722	1341	1363	1388	rBV2	598920	1533813	100.00%	13.275%
24	5.822	1392	1394	1400	rVV2	636	630	0.04%	0.005%
25	5.854	1400	1404	1409	rVV	341	509	0.03%	0.004%
26	5.874	1409	1410	1412	rVV	393	178	0.01%	0.002%
27	5.890	1413	1415	1418	rVB2	258	150	0.01%	0.001%
28	5.976	1433	1442	1456	rBV5	4845	12027	0.78%	0.104%
29	6.118	1481	1486	1488	rBV2	284	299	0.02%	0.003%
30	6.250	1511	1527	1550	rBV	288796	581803	37.93%	5.036%
31	6.398	1568	1573	1574	rBB	209	126	0.01%	0.001%
32	6.420	1577	1580	1582	rBV	138	125	0.01%	0.001%
33	6.530	1603	1614	1624	rBV2	4730	8969	0.58%	0.078%
34	6.603	1630	1637	1649	rVB6	1746	3090	0.20%	0.027%
35	6.690	1649	1664	1689	rVV	334744	678628	44.24%	5.874%
36	6.806	1694	1700	1706	rBV2	960	1204	0.08%	0.010%

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 Title : VOC Analysis

37	6.841	1706	1711	1715	rVB3	281	363	0.02%	0.003%
38	6.893	1725	1727	1730	rBV	139	121	0.01%	0.001%
39	7.086	1786	1787	1791	rVB	257	137	0.01%	0.001%
40	7.108	1792	1794	1799	rBV	261	216	0.01%	0.002%
41	7.156	1805	1809	1812	rBB	157	149	0.01%	0.001%
42	7.195	1817	1821	1824	rVV2	284	256	0.02%	0.002%
43	7.224	1828	1830	1831	rBV	380	169	0.01%	0.001%
44	7.234	1831	1833	1837	rVV3	285	220	0.01%	0.002%
45	7.427	1888	1893	1895	rBV	133	166	0.01%	0.001%
46	7.568	1924	1937	1960	rBV	194326	376502	24.55%	3.259%
47	7.690	1973	1975	1980	rVB2	377	230	0.01%	0.002%
48	7.735	1986	1989	1994	rVB	165	183	0.01%	0.002%
49	7.790	1995	2006	2019	rBV4	2085	4151	0.27%	0.036%
50	7.899	2026	2040	2057	rBV	731351	1360268	88.69%	11.773%
51	8.182	2114	2128	2154	rVV	117548	253354	16.52%	2.193%
52	8.472	2213	2218	2226	rVB	240	363	0.02%	0.003%
53	8.571	2244	2249	2257	rBV	189	379	0.02%	0.003%
54	8.677	2258	2282	2309	rBV	242805	773782	50.45%	6.697%
55	8.954	2357	2368	2378	rVV2	1372	2477	0.16%	0.021%
56	9.214	2446	2449	2454	rVB2	636	576	0.04%	0.005%
57	9.282	2467	2470	2472	rBV	177	156	0.01%	0.001%
58	9.295	2472	2474	2479	rVV	242	198	0.01%	0.002%
59	9.336	2480	2487	2492	rVB2	608	632	0.04%	0.005%
60	9.423	2500	2514	2540	rBV	348914	741440	48.34%	6.417%
61	9.542	2547	2551	2552	rBV	218	129	0.01%	0.001%
62	9.574	2552	2561	2571	rVV2	4607	8019	0.52%	0.069%
63	9.697	2587	2599	2608	rBV	16187	30081	1.96%	0.260%
64	9.742	2608	2613	2625	rVB4	6063	9416	0.61%	0.081%
65	10.018	2692	2699	2709	rBV5	1878	3048	0.20%	0.026%
66	10.115	2718	2729	2736	rBV8	3988	7549	0.49%	0.065%
67	10.166	2742	2745	2757	rVB4	1109	1232	0.08%	0.011%
68	10.250	2757	2771	2781	rBV5	4508	7850	0.51%	0.068%
69	10.314	2786	2791	2794	rBV3	918	896	0.06%	0.008%
70	10.356	2796	2804	2812	rVV7	2235	4344	0.28%	0.038%
71	10.394	2812	2816	2826	rVB3	2084	2881	0.19%	0.025%
72	10.462	2831	2837	2840	rBV4	858	997	0.07%	0.009%
73	10.555	2853	2866	2875	rBV6	3554	7435	0.48%	0.064%
74	10.626	2877	2888	2892	rBV3	4745	7964	0.52%	0.069%
75	10.771	2915	2933	2949	rBV	468266	801204	52.24%	6.934%
76	11.002	3000	3005	3008	rBV3	2880	3137	0.20%	0.027%

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 Title : VOC Analysis

77	11.063	3019	3024	3029	rBV4	2690	3223	0.21%	0.028%
78	11.115	3032	3040	3056	rVB	40986	64252	4.19%	0.556%
79	11.198	3060	3066	3073	rBV7	1414	2464	0.16%	0.021%
80	11.307	3091	3100	3109	rBV7	4393	8826	0.58%	0.076%
81	11.417	3128	3134	3140	rVV2	9196	11410	0.74%	0.099%
82	11.468	3142	3150	3166	rVB2	12549	28800	1.88%	0.249%
83	11.574	3174	3183	3191	rBV3	4868	8485	0.55%	0.073%
84	11.703	3214	3223	3231	rBV6	7319	13874	0.90%	0.120%
85	11.819	3247	3259	3271	rBV	496580	790646	51.55%	6.843%
86	11.909	3283	3287	3294	rVB7	6247	6890	0.45%	0.060%
87	12.198	3365	3377	3390	rVB	772637	1248371	81.39%	10.805%
88	12.327	3408	3417	3429	rBV	45598	65517	4.27%	0.567%
89	13.430	3752	3760	3769	rBV2	19057	28354	1.85%	0.245%
90	13.844	3883	3889	3890	rBV4	1668	1579	0.10%	0.014%
91	14.047	3944	3952	3956	rBV9	3627	5640	0.37%	0.049%
92	14.089	3957	3965	3976	rVB	24839	39796	2.59%	0.344%
93	14.449	4071	4077	4085	rVB2	12586	15925	1.04%	0.138%
94	15.137	4287	4291	4294	rBV5	1678	1686	0.11%	0.015%
95	15.224	4307	4318	4329	rBV	40053	66001	4.30%	0.571%
96	15.336	4350	4353	4355	rBV3	1360	1132	0.07%	0.010%
97	15.404	4366	4374	4387	rBV2	24807	41459	2.70%	0.359%
98	15.950	4536	4544	4559	rBV	11805	21447	1.40%	0.186%
99	16.146	4600	4605	4612	rBV6	3168	4445	0.29%	0.038%
100	16.265	4634	4642	4646	rBV2	10523	15703	1.02%	0.136%

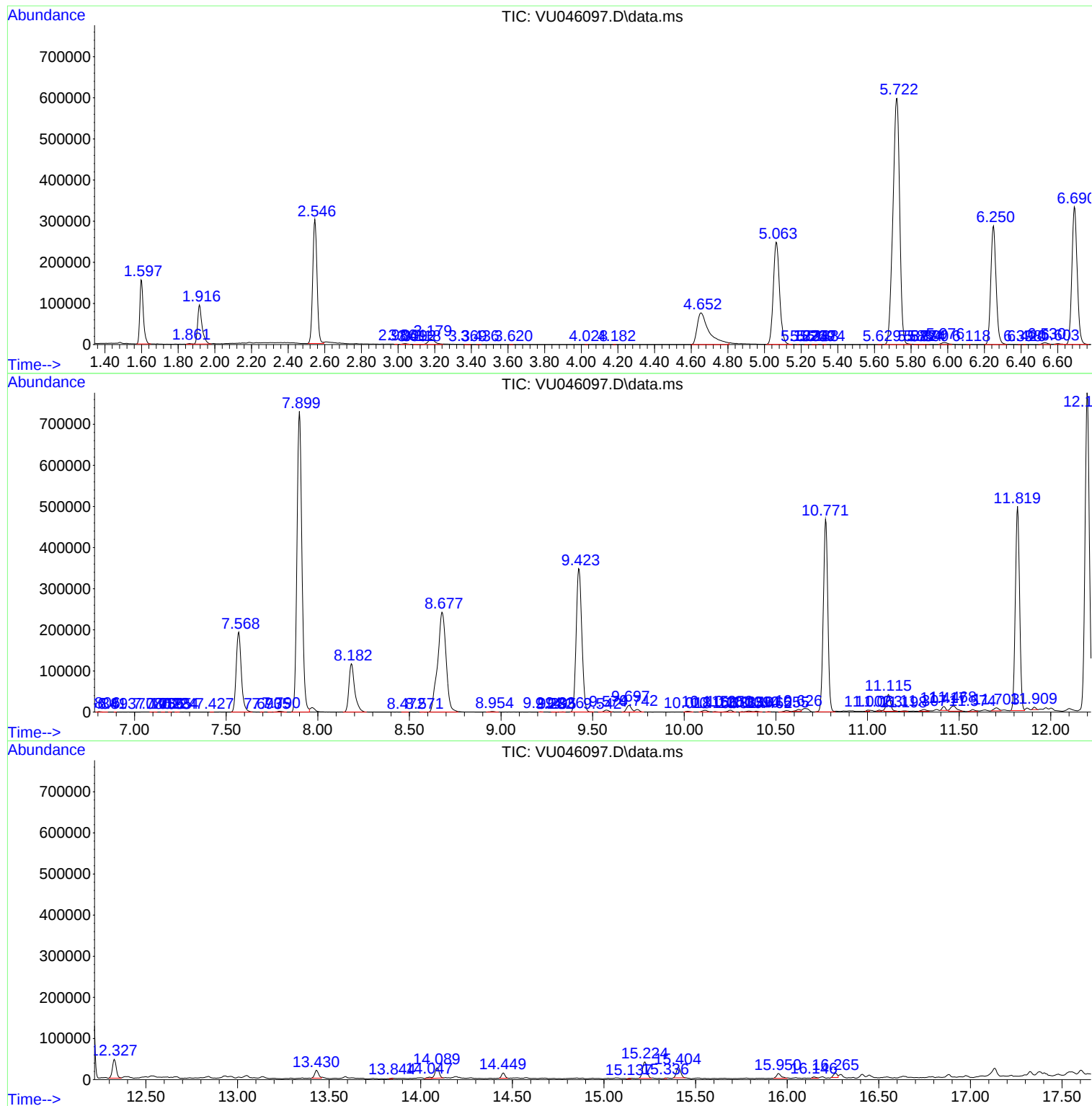
Sum of corrected areas: 11553892

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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



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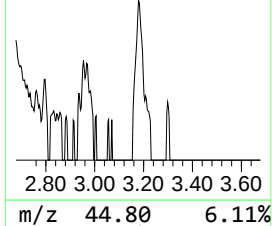
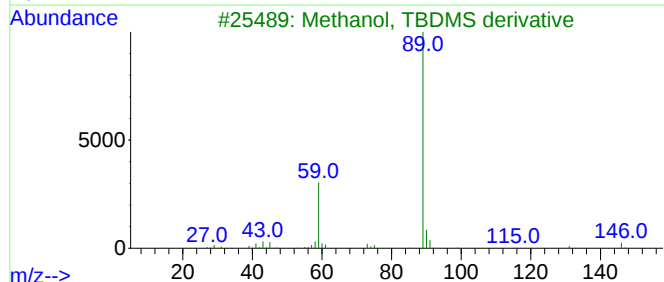
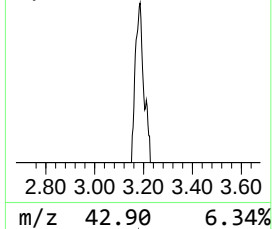
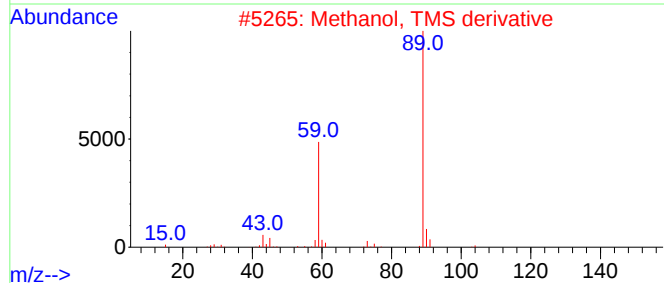
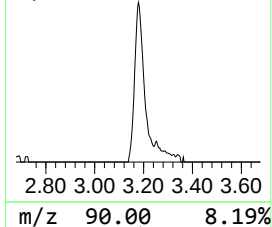
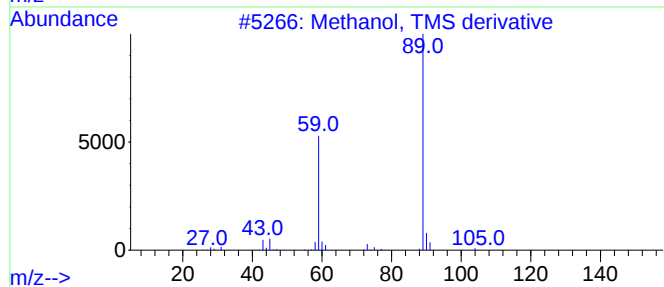
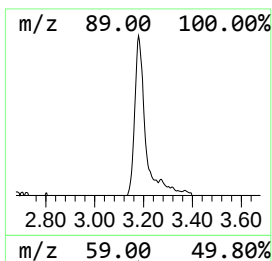
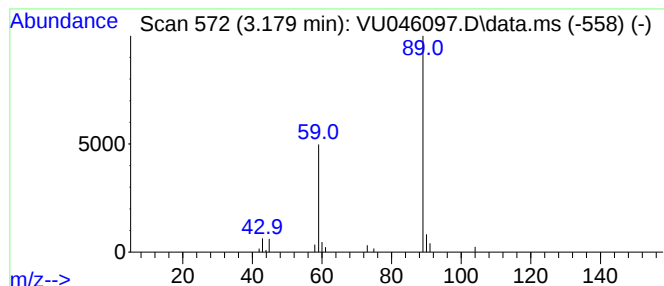
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Methanol, TMS derivative Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.179	2.85 ug/L	33212	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanol, TMS derivative	104	C4H12OSi	001825-61-2	90
2			Methanol, TMS derivative	104	C4H12OSi	001825-61-2	83
3			Methanol, TBDMS derivative	146	C7H18OSi	1000364-10-7	83
4			Ethyl(dimethyl)methoxysilane	118	C5H14OSi	052686-75-6	74
5			Silane, (2-methoxyethyl)trimethyl-	132	C6H16OSi	018173-63-2	64



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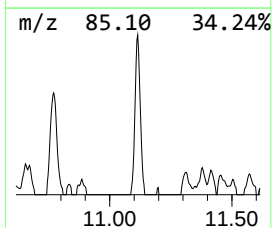
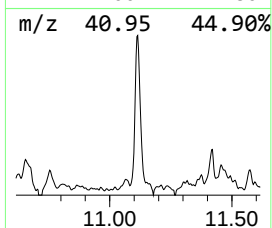
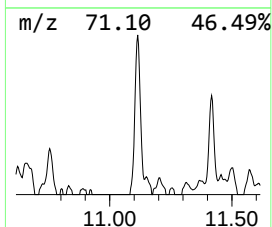
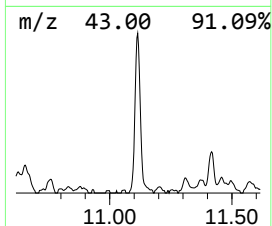
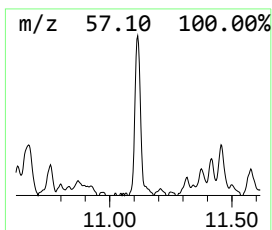
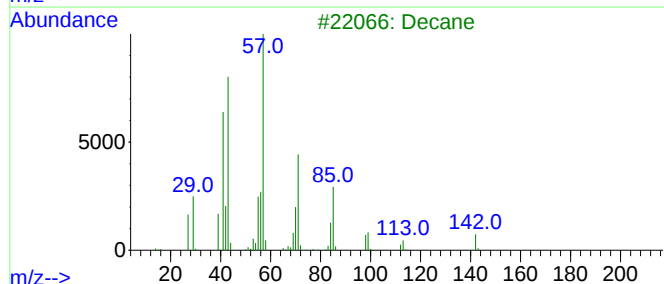
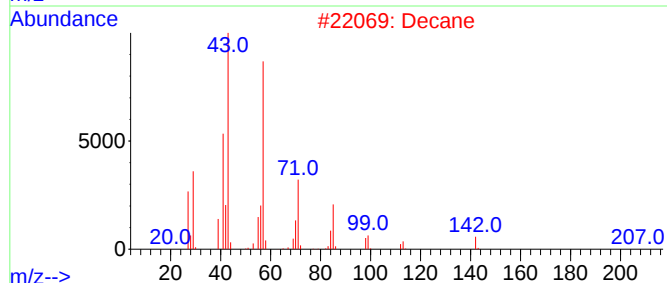
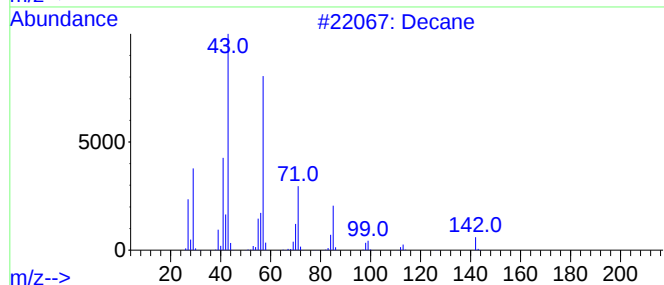
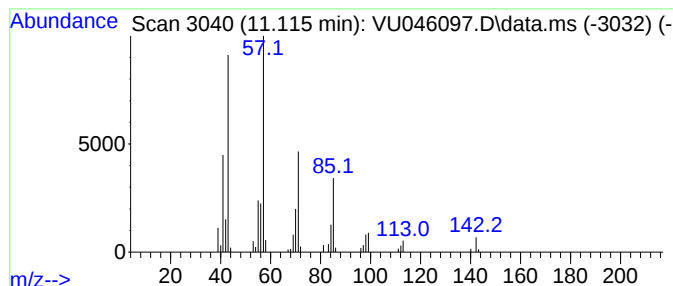
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.115	4.06 ug/L	64252	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane	142	C10H22	000124-18-5	95
2			Decane	142	C10H22	000124-18-5	95
3			Decane	142	C10H22	000124-18-5	94
4			Decane	142	C10H22	000124-18-5	91
5			Tetradecane	198	C14H30	000629-59-4	80



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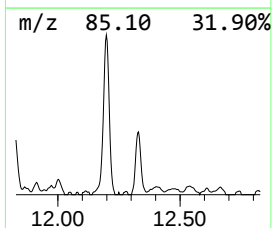
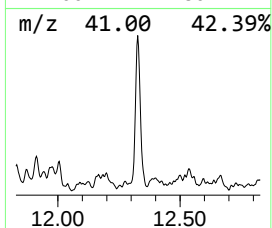
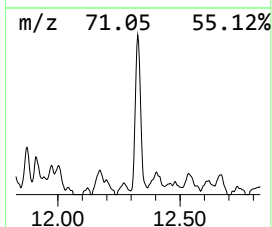
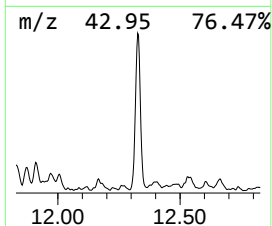
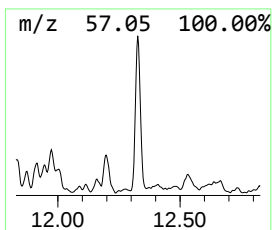
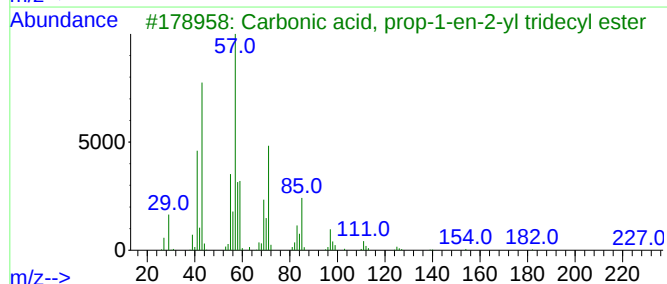
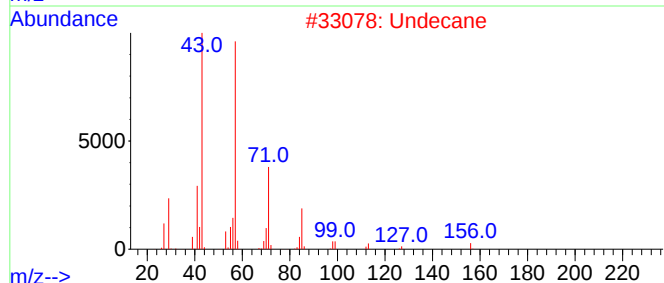
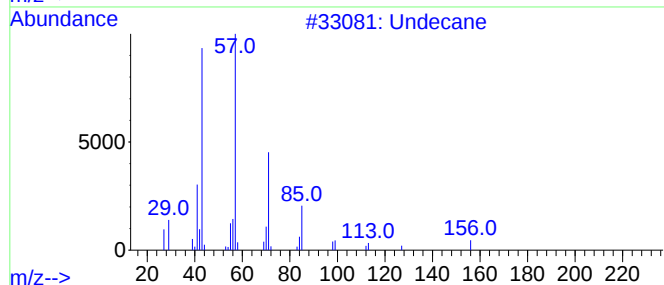
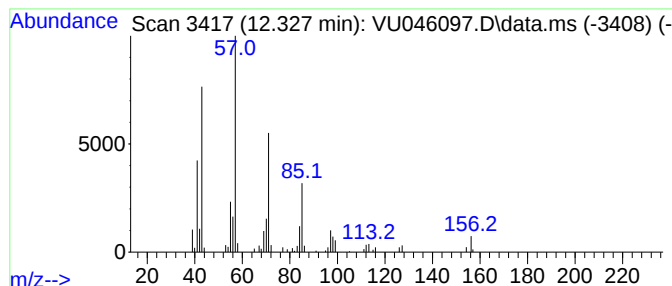
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.327	4.14 ug/L	65517	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	90
2	Undecane			156	C11H24	001120-21-4	87
3	Carbonic acid, prop-1-en-2-yl tr...			284	C17H32O3	1000382-90-8	86
4	Undecane			156	C11H24	001120-21-4	83
5	Undecane			156	C11H24	001120-21-4	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120421\
Data File : VU046097.D
Acq On : 04 Dec 2021 16:43
Operator : SY/MD
Sample : M4942-09
Misc : 6.84g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGKR1

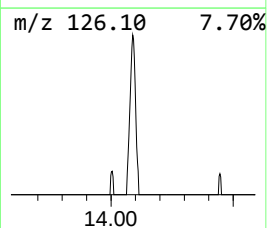
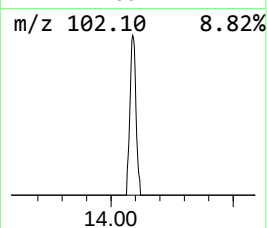
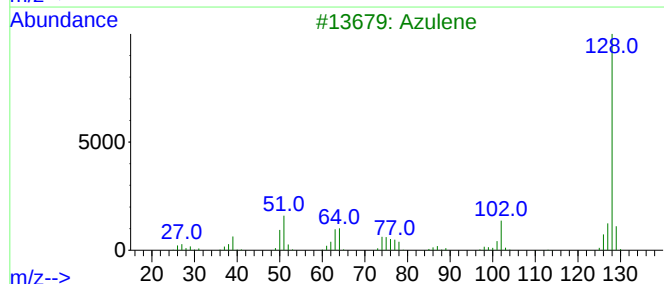
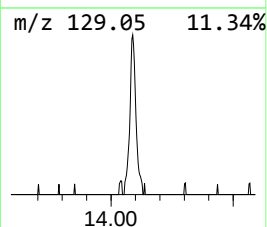
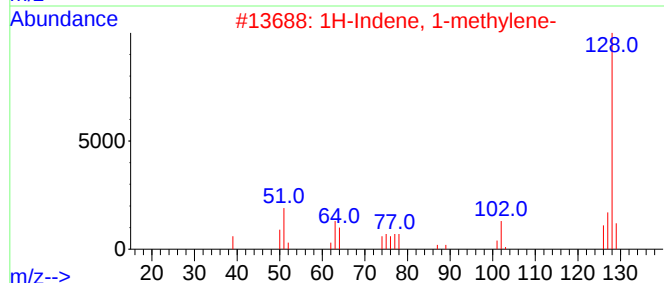
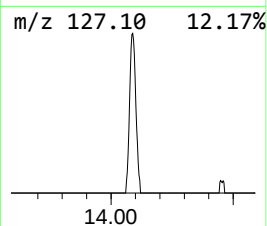
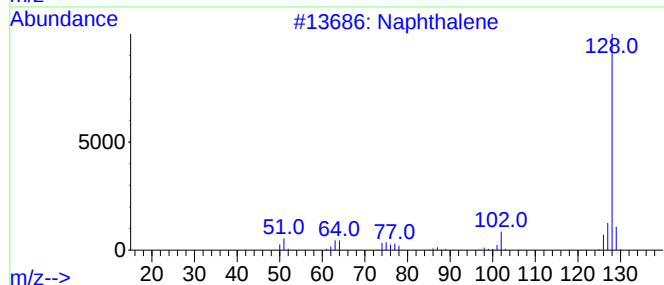
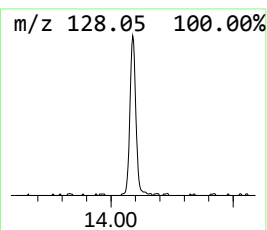
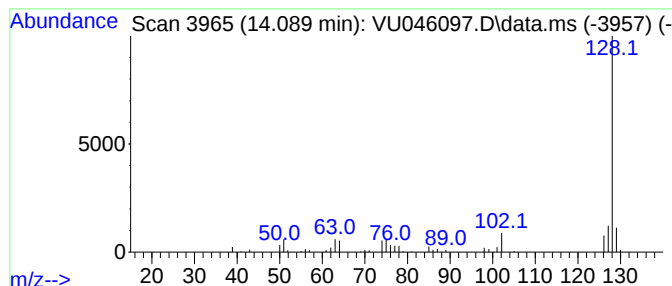
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Quant Title : VOC Analysis

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

Peak Number 5 Azulene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.089	2.52 ug/L	39796	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	93
3			Azulene	128	C10H8	000275-51-4	91
4			Azulene	128	C10H8	000275-51-4	91
5			Azulene	128	C10H8	000275-51-4	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120421\
Data File : VU046097.D
Acq On : 04 Dec 2021 16:43
Operator : SY/MD
Sample : M4942-09
Misc : 6.84g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGKR1

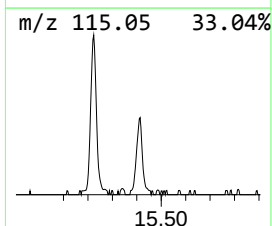
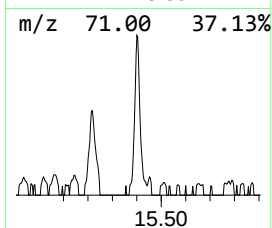
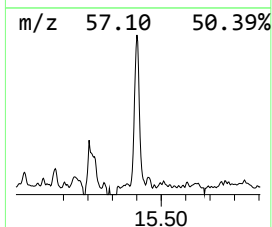
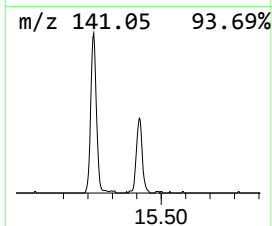
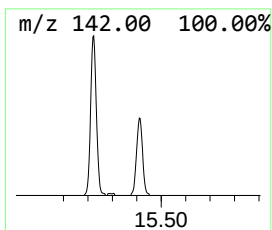
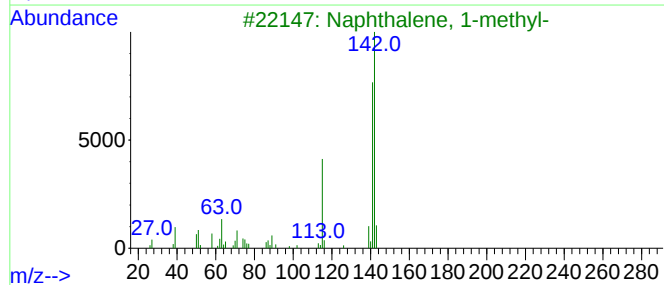
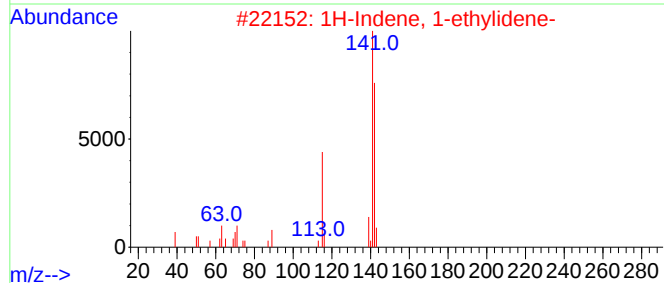
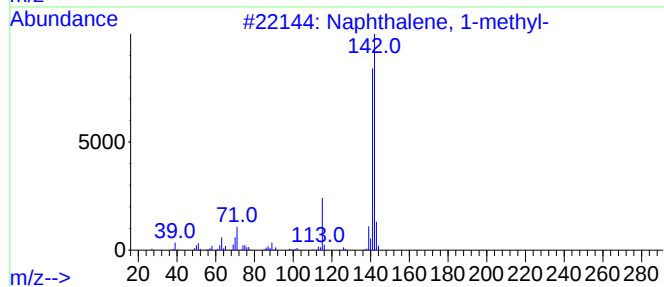
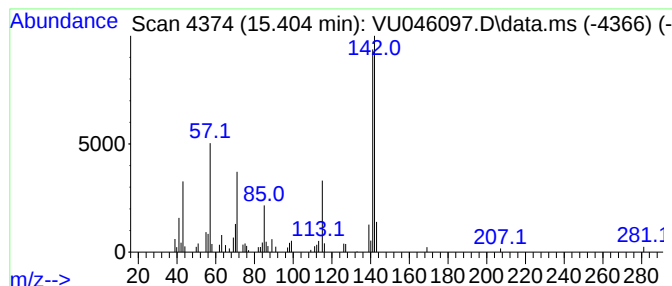
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 7 1H-Indene, 1-ethylidene- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.404	2.62 ug/L	41459	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	87
2			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	87
3			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	81
4			Benzocycloheptatriene	142	C11H10	000264-09-5	81
5			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120421\
Data File : VU046097.D
Acq On : 04 Dec 2021 16:43
Operator : SY/MD
Sample : M4942-09
Misc : 6.84g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGKR1

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
Methanol, TMS d...	3.179	2.9	ug/L	33212	1	6.250	581803	50.0
(DEL) Alkane: S...	11.115	4.1	ug/L	64252	3	11.819	790646	50.0
(DEL) Alkane: S...	12.327	4.1	ug/L	65517	3	11.819	790646	50.0
Azulene	14.089	2.5	ug/L	39796	3	11.819	790646	50.0
1H-Indene, 1-et...	15.404	2.6	ug/L	41459	3	11.819	790646	50.0