

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
 Data File : VU046143.D
 Acq On : 07 Dec 2021 16:10
 Operator : SY/MD
 Sample : M4960-04 10X
 Misc : 6.90g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 17 Sample Multiplier: 1

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: VU046143.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	74	81	94	rVB	122516	135831	14.92%	1.589%
2	1.919	171	180	197	rVB	84243	109588	12.04%	1.282%
3	2.086	228	232	234	rBV3	700	531	0.06%	0.006%
4	2.568	370	382	400	rBV	197167	328079	36.04%	3.837%
5	2.797	447	453	458	rBV	289	378	0.04%	0.004%
6	3.051	523	532	541	rVB5	1100	1870	0.21%	0.022%
7	3.189	562	575	597	rVB	10992	25732	2.83%	0.301%
8	4.642	1011	1027	1066	rBV	69589	231863	25.47%	2.712%
9	5.067	1142	1159	1183	rBV	148197	345059	37.90%	4.036%
10	5.729	1341	1365	1391	rBV2	335921	910401	100.00%	10.648%
11	6.041	1458	1462	1467	rBB	488	471	0.05%	0.006%
12	6.137	1488	1492	1497	rVB2	488	434	0.05%	0.005%
13	6.250	1512	1527	1544	rBV	265414	492999	54.15%	5.766%
14	6.536	1607	1616	1628	rVB6	2715	4753	0.52%	0.056%
15	6.694	1649	1665	1685	rBV	204002	392316	43.09%	4.589%
16	7.041	1769	1773	1781	rVB3	347	453	0.05%	0.005%
17	7.182	1811	1817	1823	rBB	401	618	0.07%	0.007%
18	7.568	1924	1937	1953	rBV	120252	207237	22.76%	2.424%
19	7.658	1963	1965	1968	rVV	493	341	0.04%	0.004%
20	7.790	1999	2006	2013	rVV3	1148	1808	0.20%	0.021%
21	7.899	2023	2040	2053	rBV	447471	762761	83.78%	8.921%
22	7.970	2054	2062	2077	rVB	38225	65903	7.24%	0.771%
23	8.131	2107	2112	2116	rBV3	621	647	0.07%	0.008%
24	8.179	2116	2127	2145	rVV	81180	136028	14.94%	1.591%
25	8.272	2154	2156	2162	rVB2	375	322	0.04%	0.004%
26	8.552	2239	2243	2251	rVB4	962	1158	0.13%	0.014%
27	8.636	2256	2269	2299	rBV	255473	471756	51.82%	5.518%
28	8.771	2308	2311	2316	rVB3	657	604	0.07%	0.007%
29	8.915	2348	2356	2365	rBV5	1562	2674	0.29%	0.031%
30	9.054	2396	2399	2405	rVB2	391	506	0.06%	0.006%
31	9.214	2442	2449	2456	rVB3	1534	2174	0.24%	0.025%
32	9.340	2480	2488	2499	rVB6	1528	2178	0.24%	0.025%
33	9.417	2499	2512	2534	rBV	374910	619577	68.06%	7.247%
34	9.571	2549	2560	2573	rBV	19645	30612	3.36%	0.358%
35	9.694	2586	2598	2608	rVV	68227	115041	12.64%	1.346%
36	9.745	2610	2614	2626	rVB2	7937	11130	1.22%	0.130%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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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

37	10.022	2693	2700	2709	rBV6	1937	3201	0.35%	0.037%
38	10.102	2713	2725	2739	rBV4	23967	44152	4.85%	0.516%
39	10.169	2744	2746	2755	rVB4	627	578	0.06%	0.007%
40	10.250	2760	2771	2784	rVB5	3755	6668	0.73%	0.078%
41	10.321	2787	2793	2796	rBV	407	393	0.04%	0.005%
42	10.356	2796	2804	2811	rBV8	3470	5578	0.61%	0.065%
43	10.388	2811	2814	2831	rVB5	1796	2893	0.32%	0.034%
44	10.485	2834	2844	2853	rVB2	7758	11701	1.29%	0.137%
45	10.568	2858	2870	2880	rBV3	16423	28247	3.10%	0.330%
46	10.626	2882	2888	2891	rBV4	2648	3066	0.34%	0.036%
47	10.758	2914	2929	2956	rBV	304478	493352	54.19%	5.770%
48	10.864	2958	2962	2965	rVV2	954	903	0.10%	0.011%
49	10.906	2968	2975	2987	rVB2	5794	9494	1.04%	0.111%
50	10.999	2994	3004	3011	rBV2	19616	35430	3.89%	0.414%
51	11.115	3027	3040	3058	rVB3	32844	68120	7.48%	0.797%
52	11.205	3063	3068	3076	rVB3	1258	1458	0.16%	0.017%
53	11.243	3076	3080	3086	rBV2	832	747	0.08%	0.009%
54	11.295	3086	3096	3114	rBV	8628	19959	2.19%	0.233%
55	11.375	3115	3121	3126	rVV6	3227	4940	0.54%	0.058%
56	11.417	3127	3134	3140	rVV4	8967	13745	1.51%	0.161%
57	11.468	3140	3150	3167	rVB	44096	73781	8.10%	0.863%
58	11.575	3176	3183	3190	rBV5	3590	5971	0.66%	0.070%
59	11.642	3199	3204	3212	rVB5	3071	4451	0.49%	0.052%
60	11.706	3214	3224	3231	rBV8	6458	12590	1.38%	0.147%
61	11.812	3245	3257	3270	rBV	448798	699719	76.86%	8.184%
62	11.896	3271	3283	3294	rVV4	10779	25950	2.85%	0.304%
63	12.099	3339	3346	3350	rBV4	5658	7588	0.83%	0.089%
64	12.192	3362	3375	3391	rVB	476375	792637	87.06%	9.271%
65	12.327	3407	3417	3427	rBV2	43299	61796	6.79%	0.723%
66	12.382	3429	3434	3440	rBV4	3266	4224	0.46%	0.049%
67	12.472	3453	3462	3464	rBV4	4191	6259	0.69%	0.073%
68	12.774	3552	3556	3561	rBV4	930	1065	0.12%	0.012%
69	12.877	3582	3588	3590	rBV5	1514	1487	0.16%	0.017%
70	12.925	3597	3603	3604	rBV4	3016	2655	0.29%	0.031%
71	13.134	3663	3668	3675	rVB5	3358	3775	0.41%	0.044%
72	13.266	3702	3709	3714	rBV4	5175	8363	0.92%	0.098%
73	13.353	3729	3736	3743	rBV7	1973	2734	0.30%	0.032%
74	13.433	3752	3761	3781	rVB4	25212	50443	5.54%	0.590%
75	13.584	3804	3808	3815	rVB2	4701	5322	0.58%	0.062%
76	13.732	3846	3854	3860	rBV7	1455	2454	0.27%	0.029%

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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

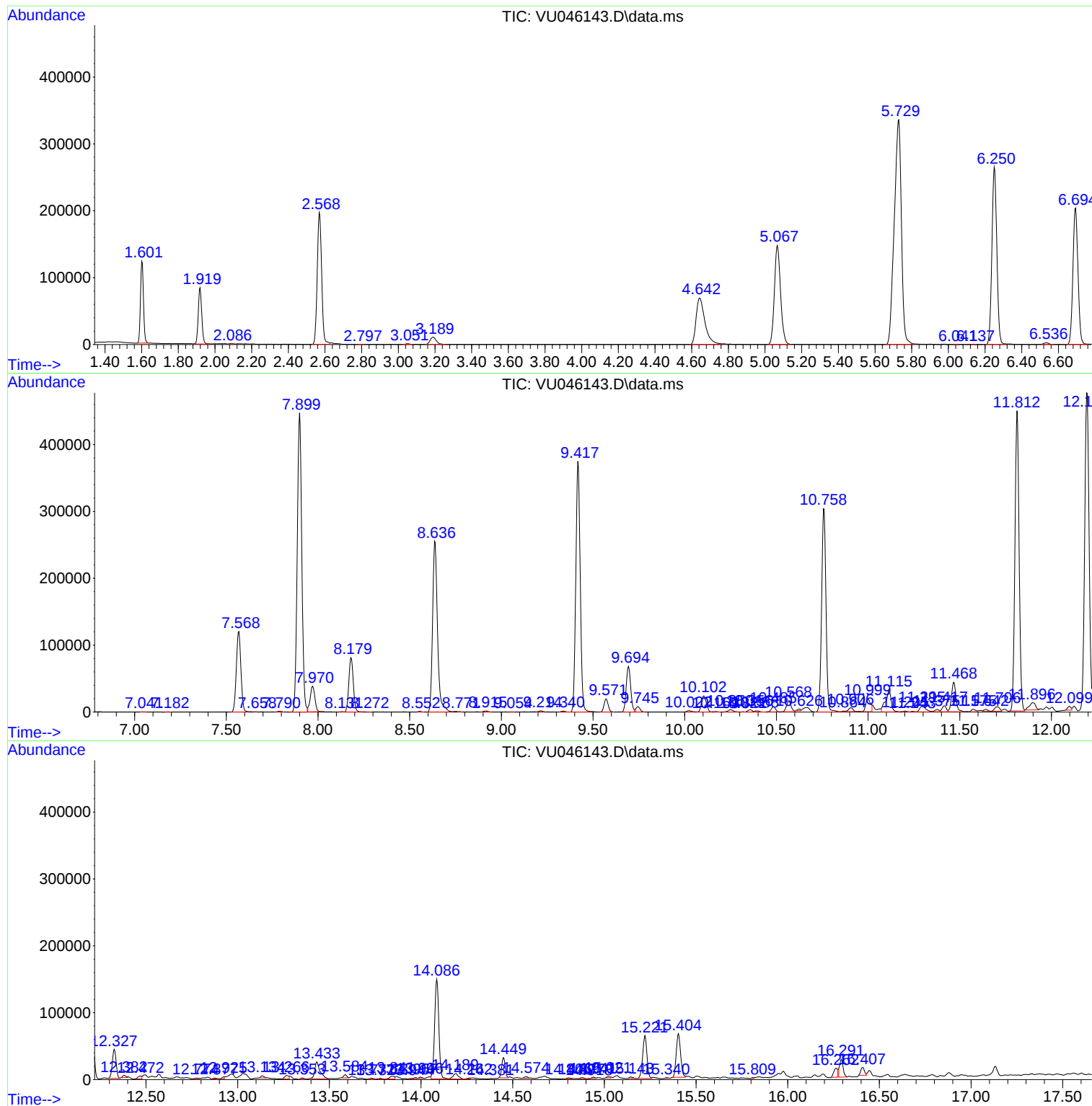
77	13.777	3865	3868	3877	rVB3	1001	1114	0.12%	0.013%
78	13.841	3878	3888	3893	rBV7	4087	7675	0.84%	0.090%
79	13.944	3916	3920	3922	rBV3	758	642	0.07%	0.008%
80	13.967	3922	3927	3931	rVV5	1735	2024	0.22%	0.024%
81	13.996	3934	3936	3943	rVB5	2187	2170	0.24%	0.025%
82	14.086	3954	3964	3985	rVB	148906	236374	25.96%	2.765%
83	14.189	3986	3996	4010	rVB6	8407	17233	1.89%	0.202%
84	14.262	4010	4019	4021	rBV5	1609	1988	0.22%	0.023%
85	14.381	4053	4056	4057	rBV2	706	480	0.05%	0.006%
86	14.449	4069	4077	4085	rBV	30287	39543	4.34%	0.462%
87	14.574	4110	4116	4122	rBV6	2159	2912	0.32%	0.034%
88	14.806	4182	4188	4194	rBV9	1848	3004	0.33%	0.035%
89	14.877	4206	4210	4218	rVB6	1715	2426	0.27%	0.028%
90	14.918	4220	4223	4224	rBV2	640	365	0.04%	0.004%
91	14.941	4225	4230	4234	rBV6	2006	2291	0.25%	0.027%
92	15.021	4250	4255	4259	rBV7	2335	2666	0.29%	0.031%
93	15.143	4288	4293	4303	rVB8	2286	3394	0.37%	0.040%
94	15.221	4305	4317	4329	rBV	63841	103432	11.36%	1.210%
95	15.340	4351	4354	4357	rBV5	994	820	0.09%	0.010%
96	15.404	4364	4374	4386	rBV2	65329	106910	11.74%	1.250%
97	15.809	4496	4500	4502	rBV4	1375	1184	0.13%	0.014%
98	16.262	4633	4641	4644	rBV3	13408	19063	2.09%	0.223%
99	16.291	4646	4650	4661	rVB	26478	34175	3.75%	0.400%
100	16.407	4680	4686	4693	rBV3	11693	16347	1.80%	0.191%

Sum of corrected areas: 8549954

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ALS Vial : 17 Sample Multiplier: 1

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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ALS Vial : 17 Sample Multiplier: 1

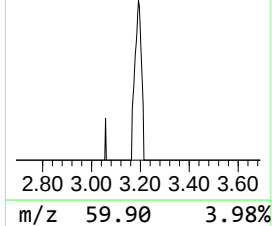
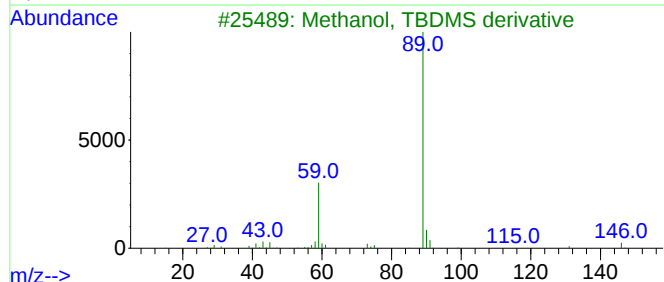
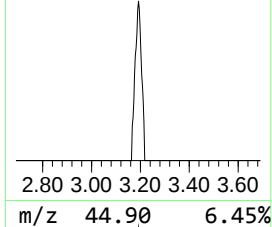
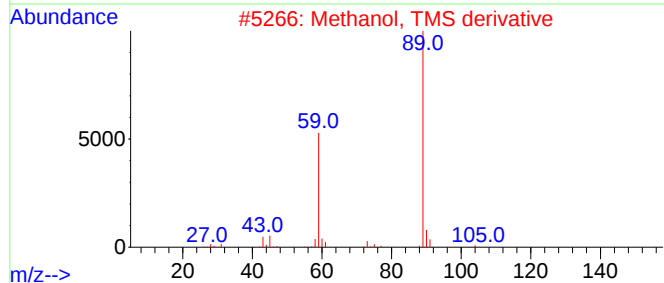
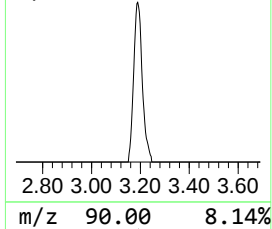
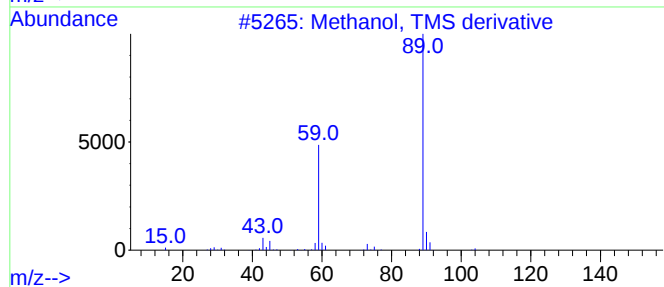
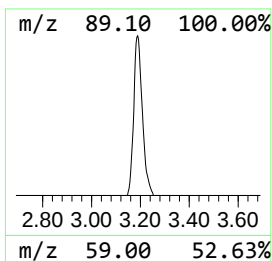
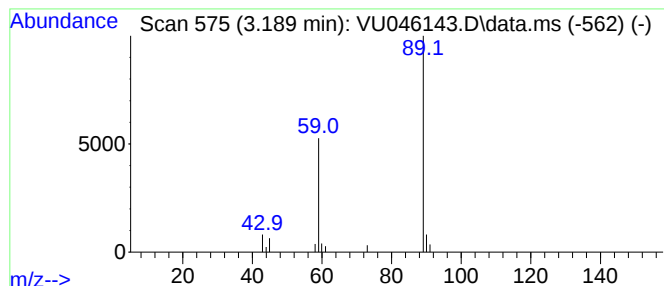
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Methanol, TMS derivative Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.189	2.61 ug/L	25732	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanol, TMS derivative	104	C4H12OSi	001825-61-2	83
2			Methanol, TMS derivative	104	C4H12OSi	001825-61-2	83
3			Methanol, TBDMS derivative	146	C7H18OSi	1000364-10-7	74
4			Silane, (2-methoxyethyl)trimethyl-	132	C6H16OSi	018173-63-2	74
5			Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	9



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ALS Vial : 17 Sample Multiplier: 1

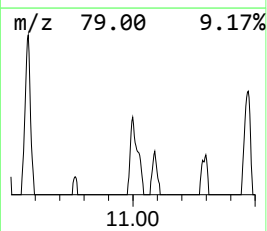
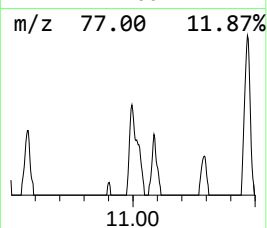
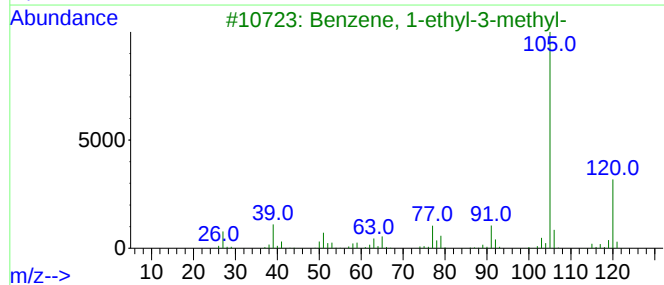
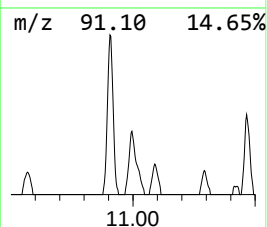
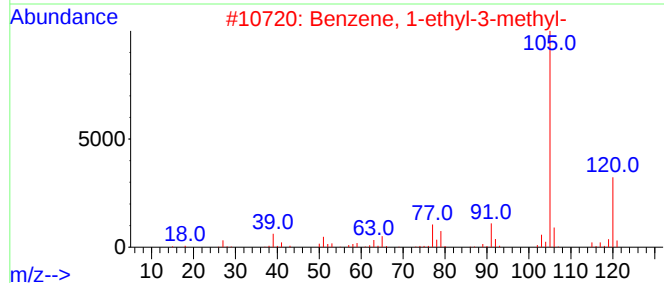
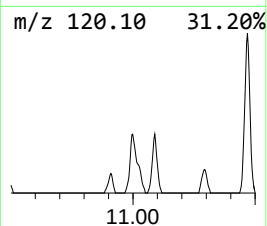
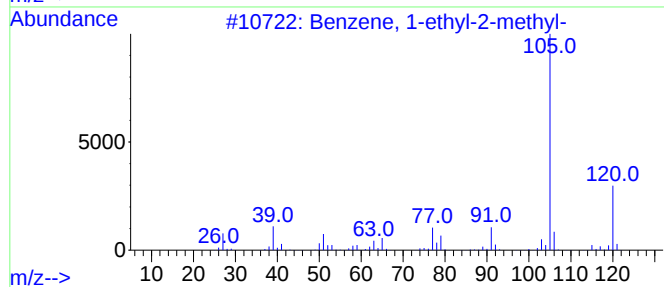
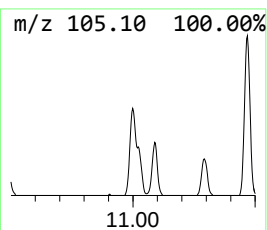
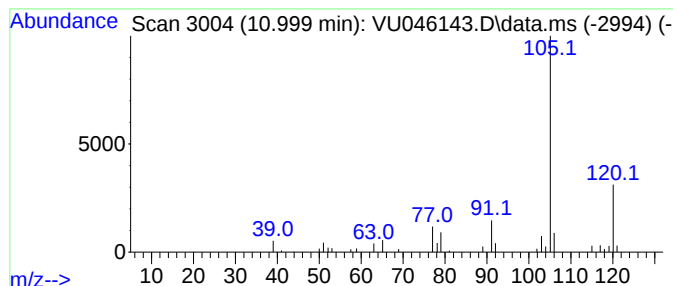
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.999	2.53 ug/L	35430	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
4			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



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ALS Vial : 17 Sample Multiplier: 1

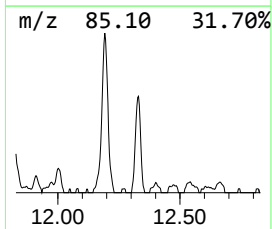
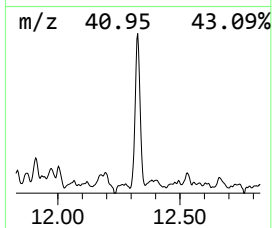
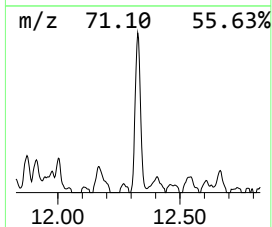
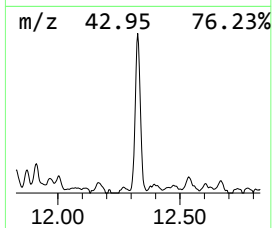
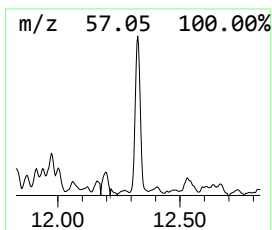
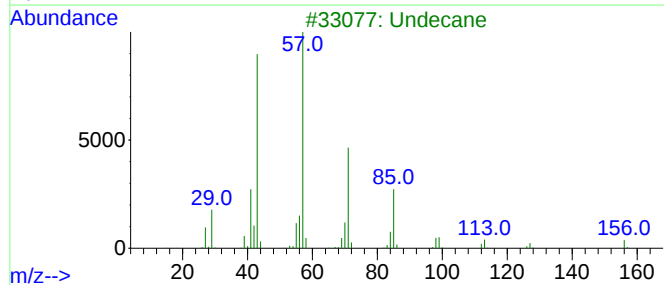
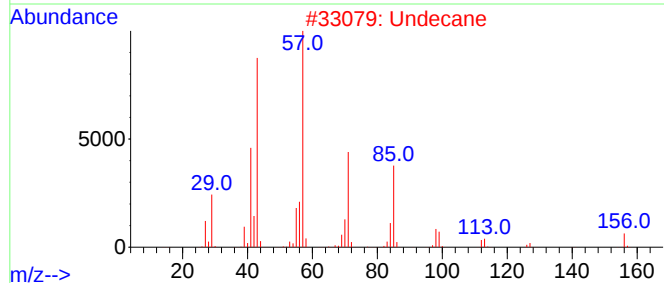
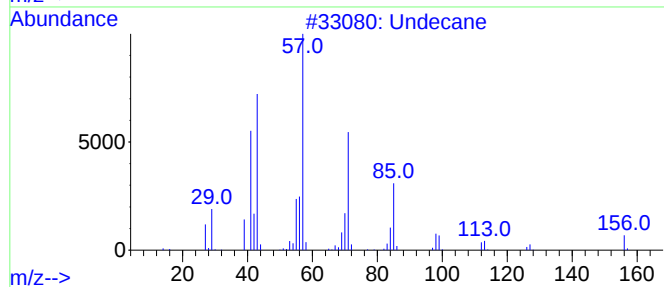
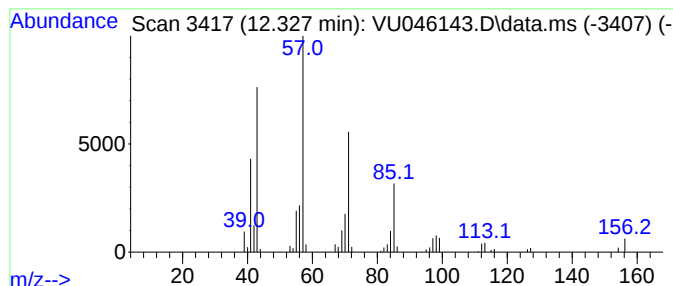
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.327	4.42 ug/L	61796	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	96
2	Undecane			156	C11H24	001120-21-4	93
3	Undecane			156	C11H24	001120-21-4	91
4	Undecane			156	C11H24	001120-21-4	87
5	Hexadecane			226	C16H34	000544-76-3	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
Data File : VU046143.D
Acq On : 07 Dec 2021 16:10
Operator : SY/MD
Sample : M4960-04 10X
Misc : 6.90g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 17 Sample Multiplier: 1

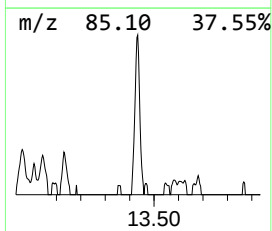
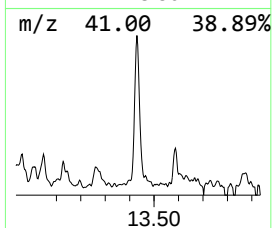
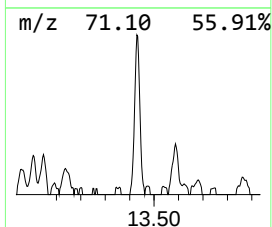
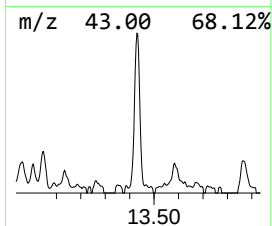
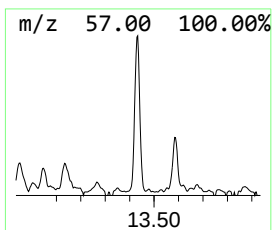
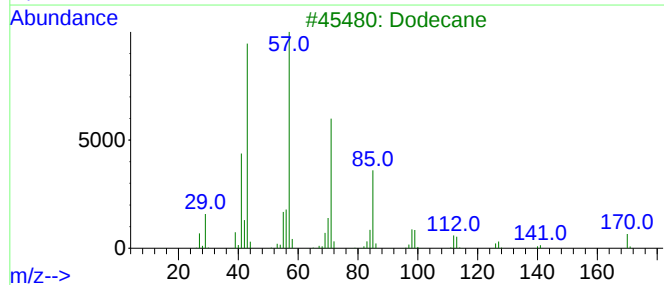
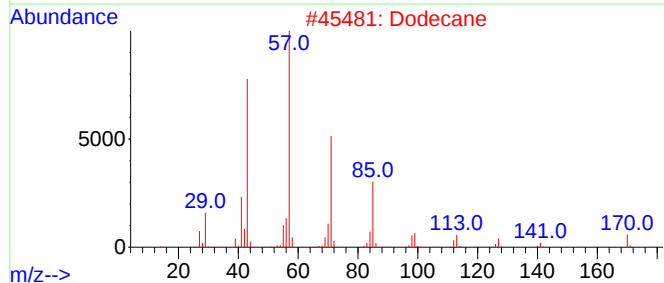
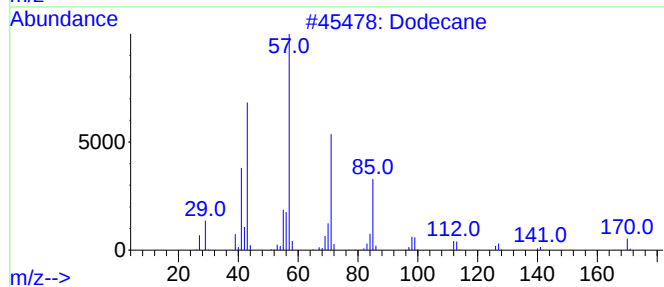
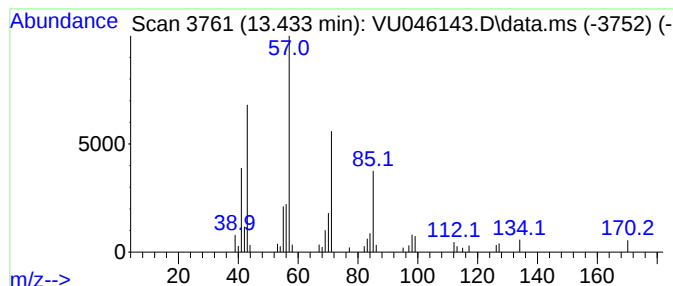
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Quant Title : VOC Analysis

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.433	3.60 ug/L	50443	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	94
2			Dodecane	170	C12H26	000112-40-3	87
3			Dodecane	170	C12H26	000112-40-3	83
4			Undecane, 2-methyl-	170	C12H26	007045-71-8	72
5			Tridecane	184	C13H28	000629-50-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
Data File : VU046143.D
Acq On : 07 Dec 2021 16:10
Operator : SY/MD
Sample : M4960-04 10X
Misc : 6.90g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 17 Sample Multiplier: 1

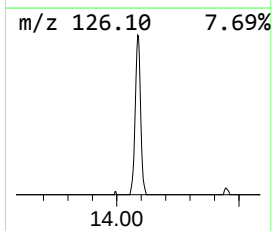
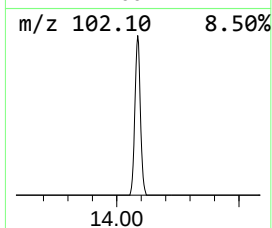
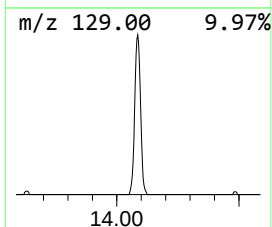
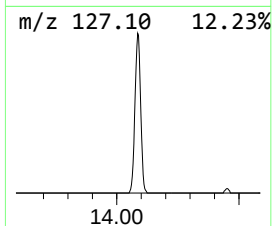
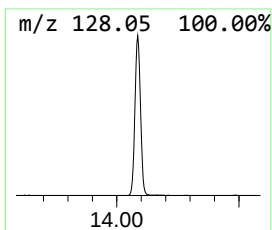
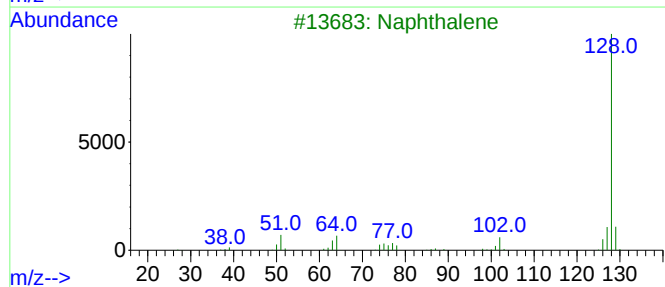
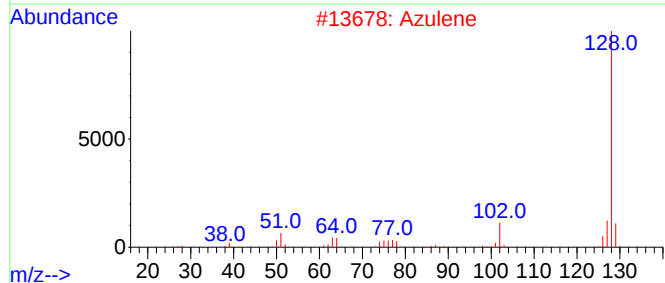
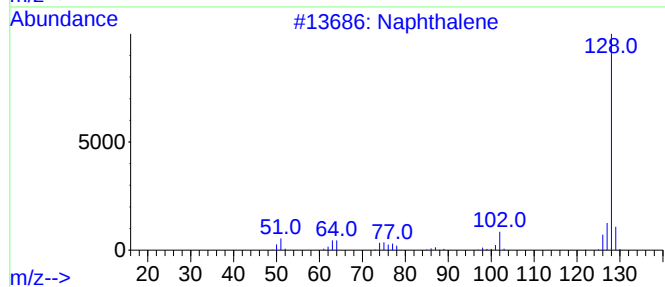
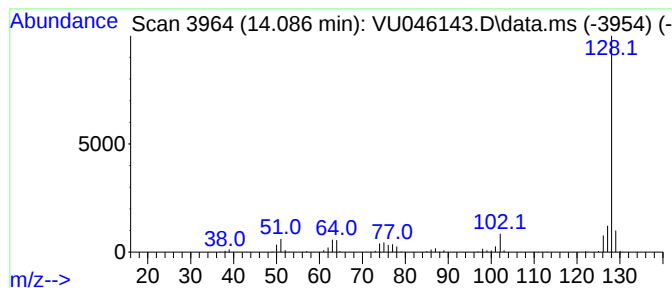
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Quant Title : VOC Analysis

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

Peak Number 6 Azulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.086	16.89 ug/L	236374	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Azulene	128	C10H8	000275-51-4	93
3			Naphthalene	128	C10H8	000091-20-3	93
4			Azulene	128	C10H8	000275-51-4	91
5			Azulene	128	C10H8	000275-51-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
Data File : VU046143.D
Acq On : 07 Dec 2021 16:10
Operator : SY/MD
Sample : M4960-04 10X
Misc : 6.90g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 17 Sample Multiplier: 1

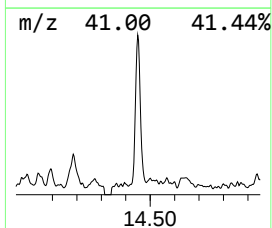
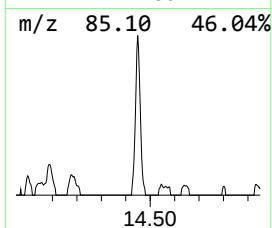
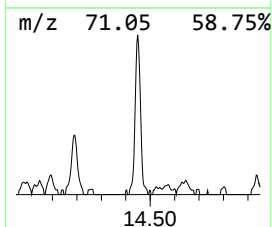
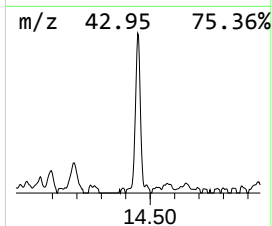
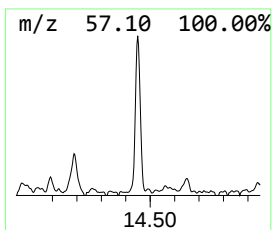
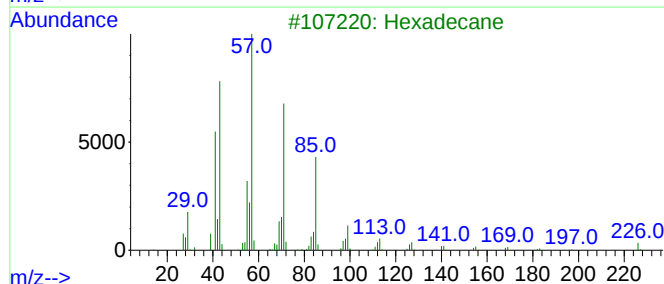
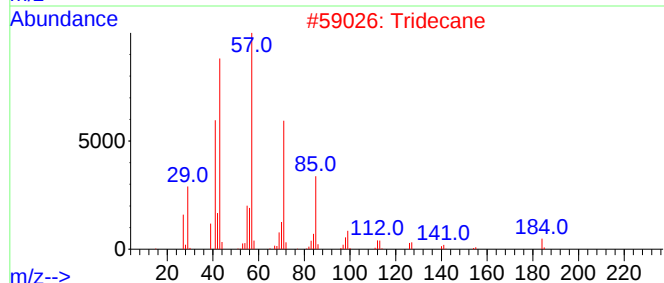
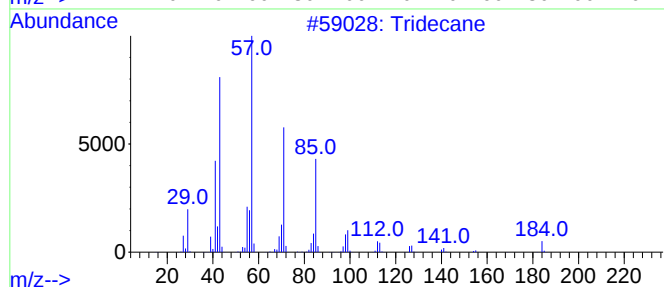
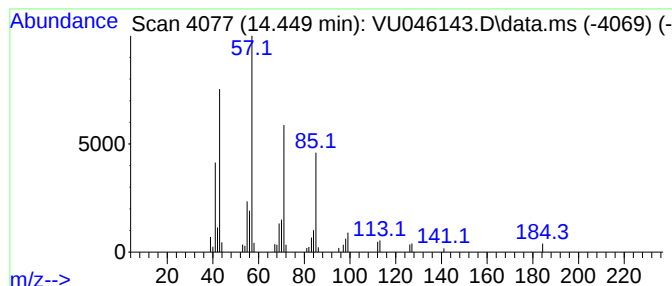
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.449	2.83 ug/L	39543	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	96
2			Tridecane	184	C13H28	000629-50-5	95
3			Hexadecane	226	C16H34	000544-76-3	90
4			Pentadecane	212	C15H32	000629-62-9	90
5			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
Data File : VU046143.D
Acq On : 07 Dec 2021 16:10
Operator : SY/MD
Sample : M4960-04 10X
Misc : 6.90g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 17 Sample Multiplier: 1

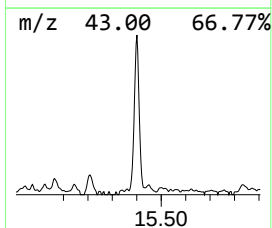
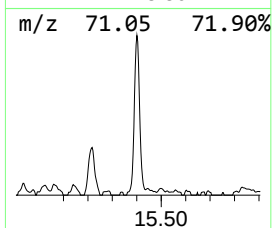
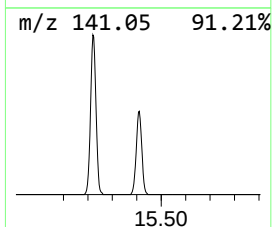
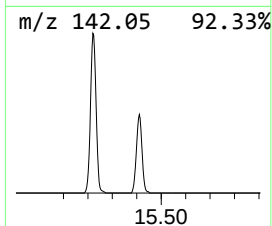
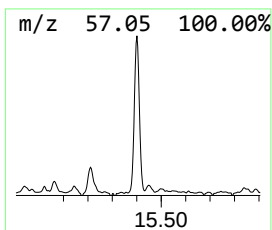
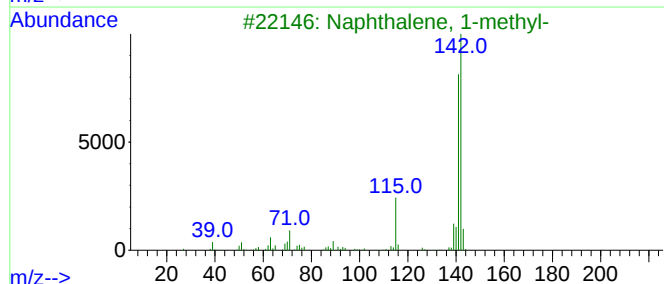
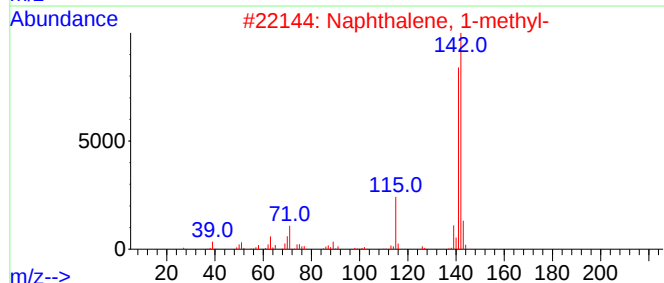
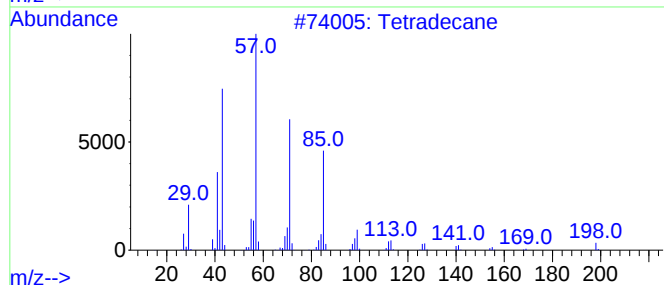
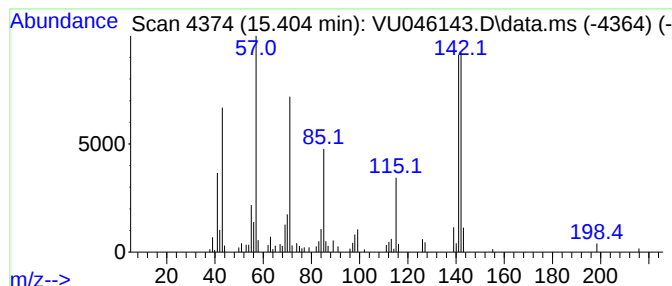
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Quant Title : VOC Analysis

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

Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.404	7.64 ug/L	106910	1,4-Dichlorobenzene-d4	11.812

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane	198	C14H30	000629-59-4	78
2		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	76
3		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	68
4		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	64
5		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
Data File : VU046143.D
Acq On : 07 Dec 2021 16:10
Operator : SY/MD
Sample : M4960-04 10X
Misc : 6.90g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 17 Sample Multiplier: 1

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Methanol, TMS d...	3.189	2.6	ug/L	25732	1	6.250	492999	50.0
Benzene, 1-ethy...	10.999	2.5	ug/L	35430	3	11.812	699719	50.0
(DEL) Alkane: S...	12.327	4.4	ug/L	61796	3	11.812	699719	50.0
(DEL) Alkane: S...	13.433	3.6	ug/L	50443	3	11.812	699719	50.0
Azulene	14.086	16.9	ug/L	236374	3	11.812	699719	50.0
(DEL) Alkane: S...	14.449	2.8	ug/L	39543	3	11.812	699719	50.0
(DEL) Alkane: S...	15.404	7.6	ug/L	106910	3	11.812	699719	50.0