

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050422\
 Data File : VU048424.D
 Acq On : 04 May 2022 19:43
 Operator : SY/MD
 Sample : N2632-14ME
 Misc : 7.49g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW4B6ME

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\SFAMULM042522WMA.M
 Title : VOC Analysis

Signal : TIC: VU048424.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.478	37	43	48	rBV2	8041	10910	0.44%	0.059%
2	1.597	73	80	116	rVB	136297	396027	15.87%	2.155%
3	1.855	155	160	163	rBV	44133	48716	1.95%	0.265%
4	2.466	347	350	353	rVB3	389	224	0.01%	0.001%
5	2.533	358	371	425	rVV	405920	827718	33.17%	4.503%
6	2.793	449	452	455	rBV2	337	218	0.01%	0.001%
7	2.839	464	466	472	rVB2	363	207	0.01%	0.001%
8	2.896	482	484	489	rVB3	484	328	0.01%	0.002%
9	2.961	495	504	512	rBV3	1564	3108	0.12%	0.017%
10	3.031	519	526	538	rVB6	2470	4925	0.20%	0.027%
11	3.179	557	572	595	rBV2	18472	49203	1.97%	0.268%
12	3.485	664	667	673	rVB2	234	223	0.01%	0.001%
13	3.591	697	700	707	rVB	278	282	0.01%	0.002%
14	3.623	707	710	714	rBV2	304	296	0.01%	0.002%
15	3.816	763	770	773	rBV2	254	324	0.01%	0.002%
16	4.375	941	944	951	rVB2	238	269	0.01%	0.001%
17	4.568	996	1004	1007	rBV2	350	412	0.02%	0.002%
18	4.639	1007	1026	1100	rBV	170075	745084	29.86%	4.054%
19	5.063	1140	1158	1188	rVV	378323	931161	37.32%	5.066%
20	5.279	1221	1225	1229	rBV3	379	382	0.02%	0.002%
21	5.356	1242	1249	1252	rBV4	549	680	0.03%	0.004%
22	5.379	1253	1256	1262	rVV4	463	364	0.01%	0.002%
23	5.575	1314	1317	1322	rVB2	211	204	0.01%	0.001%
24	5.719	1341	1362	1391	rBV2	998996	2495133	100.00%	13.575%
25	5.977	1430	1442	1458	rBV2	13260	31829	1.28%	0.173%
26	6.153	1493	1497	1499	rBV2	529	428	0.02%	0.002%
27	6.247	1512	1526	1554	rBV	420801	867174	34.75%	4.718%
28	6.443	1584	1587	1595	rVB3	317	370	0.01%	0.002%
29	6.491	1595	1602	1603	rBV3	444	373	0.01%	0.002%
30	6.523	1603	1612	1626	rVV6	6552	13571	0.54%	0.074%
31	6.600	1627	1636	1649	rVV4	6354	15239	0.61%	0.083%
32	6.690	1649	1664	1693	rVV	522527	1118766	44.84%	6.087%
33	6.806	1693	1700	1713	rVB7	2223	4301	0.17%	0.023%
34	6.858	1713	1716	1721	rVB4	305	315	0.01%	0.002%
35	6.919	1731	1735	1736	rBV2	371	221	0.01%	0.001%
36	6.961	1745	1748	1752	rBV2	356	264	0.01%	0.001%

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 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW4B6ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Start Thrs: 0.2

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\SFAMULM042522WMA.M
 Title : VOC Analysis

37	6.977	1752	1753	1757	rVB2	490	245	0.01%	0.001%
38	6.999	1757	1760	1764	rVB2	322	276	0.01%	0.002%
39	7.051	1773	1776	1778	rBV2	397	262	0.01%	0.001%
40	7.067	1778	1781	1786	rVB2	353	304	0.01%	0.002%
41	7.092	1787	1789	1794	rVB3	699	592	0.02%	0.003%
42	7.192	1809	1820	1822	rBV4	7783	11438	0.46%	0.062%
43	7.343	1866	1867	1872	rVB2	295	206	0.01%	0.001%
44	7.404	1883	1886	1892	rVB2	413	461	0.02%	0.003%
45	7.436	1892	1896	1901	rBV3	291	310	0.01%	0.002%
46	7.501	1908	1916	1923	rBV6	1177	1805	0.07%	0.010%
47	7.568	1923	1937	1961	rBV	261250	545486	21.86%	2.968%
48	7.697	1968	1977	1983	rBV4	2032	3344	0.13%	0.018%
49	7.790	1997	2006	2007	rBV4	902	1098	0.04%	0.006%
50	7.899	2025	2040	2058	rBV	1116762	2099661	84.15%	11.423%
51	8.131	2105	2112	2115	rBV4	1638	1798	0.07%	0.010%
52	8.182	2116	2128	2152	rVV	164187	367034	14.71%	1.997%
53	8.353	2174	2181	2189	rBV5	1560	2512	0.10%	0.014%
54	8.385	2189	2191	2193	rVV	525	336	0.01%	0.002%
55	8.536	2232	2238	2240	rVV5	909	837	0.03%	0.005%
56	8.549	2240	2242	2248	rVB3	679	400	0.02%	0.002%
57	8.661	2258	2277	2303	rBV	654438	1532073	61.40%	8.335%
58	8.925	2347	2359	2369	rBV4	4310	8092	0.32%	0.044%
59	8.960	2369	2370	2373	rVV2	671	295	0.01%	0.002%
60	8.986	2376	2378	2380	rVB2	567	211	0.01%	0.001%
61	9.041	2391	2395	2396	rBV2	355	239	0.01%	0.001%
62	9.063	2399	2402	2409	rVB2	784	712	0.03%	0.004%
63	9.099	2409	2413	2415	rBV2	359	326	0.01%	0.002%
64	9.115	2415	2418	2420	rVB2	499	253	0.01%	0.001%
65	9.163	2428	2433	2442	rBV6	1472	2371	0.10%	0.013%
66	9.211	2442	2448	2457	rVB5	2949	4258	0.17%	0.023%
67	9.337	2478	2487	2499	rVB3	2683	3920	0.16%	0.021%
68	9.423	2499	2514	2537	rBV	541923	1125976	45.13%	6.126%
69	9.575	2555	2561	2562	rBV2	815	731	0.03%	0.004%
70	9.658	2581	2587	2593	rBV4	1313	1979	0.08%	0.011%
71	9.697	2593	2599	2605	rVV6	1823	3215	0.13%	0.017%
72	9.742	2606	2613	2623	rVB3	7196	10862	0.44%	0.059%
73	9.864	2648	2651	2652	rBV	504	213	0.01%	0.001%
74	10.015	2692	2698	2708	rBV6	1665	2629	0.11%	0.014%
75	10.121	2720	2731	2737	rBV6	2045	3114	0.12%	0.017%
76	10.250	2753	2771	2781	rBV4	6455	11072	0.44%	0.060%

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Instrument :
 MSVOA_U
 ClientSampleId :
 EW4B6ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Start Thrs: 0.2

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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\SFAMULM042522WMA.M
 Title : VOC Analysis

77	10.298	2781	2786	2787	rBV3	429	305	0.01%	0.002%
78	10.314	2788	2791	2792	rBV3	703	319	0.01%	0.002%
79	10.340	2796	2799	2800	rBV3	551	349	0.01%	0.002%
80	10.394	2810	2816	2828	rVB4	5603	9274	0.37%	0.050%
81	10.468	2832	2839	2843	rBV5	1363	1972	0.08%	0.011%
82	10.562	2852	2868	2876	rBV8	2759	6546	0.26%	0.036%
83	10.623	2880	2887	2892	rBV5	4325	6073	0.24%	0.033%
84	10.767	2914	2932	2957	rBV	903521	1485875	59.55%	8.084%
85	11.063	3018	3024	3030	rBV7	2075	3371	0.14%	0.018%
86	11.115	3031	3040	3057	rVB2	30619	49860	2.00%	0.271%
87	11.247	3077	3081	3090	rVB7	976	1139	0.05%	0.006%
88	11.317	3091	3103	3112	rBV10	4596	8878	0.36%	0.048%
89	11.417	3127	3134	3141	rBV	20797	25727	1.03%	0.140%
90	11.574	3174	3183	3188	rBV5	3233	5644	0.23%	0.031%
91	11.819	3246	3259	3271	rBV	710432	1138985	45.65%	6.197%
92	11.912	3283	3288	3295	rBV7	5729	7077	0.28%	0.039%
93	12.086	3336	3342	3346	rBV6	2392	2971	0.12%	0.016%
94	12.198	3365	3377	3393	rVB	1154497	1868148	74.87%	10.164%
95	12.327	3408	3417	3429	rBV	81210	119967	4.81%	0.653%
96	12.664	3517	3522	3532	rVB4	10909	15586	0.62%	0.085%
97	13.047	3636	3641	3650	rVB6	11203	15422	0.62%	0.084%
98	13.433	3752	3761	3770	rBV	89796	133725	5.36%	0.728%
99	13.587	3801	3809	3818	rBV	44510	67922	2.72%	0.370%
100	14.449	4070	4077	4086	rBV	64400	85058	3.41%	0.463%

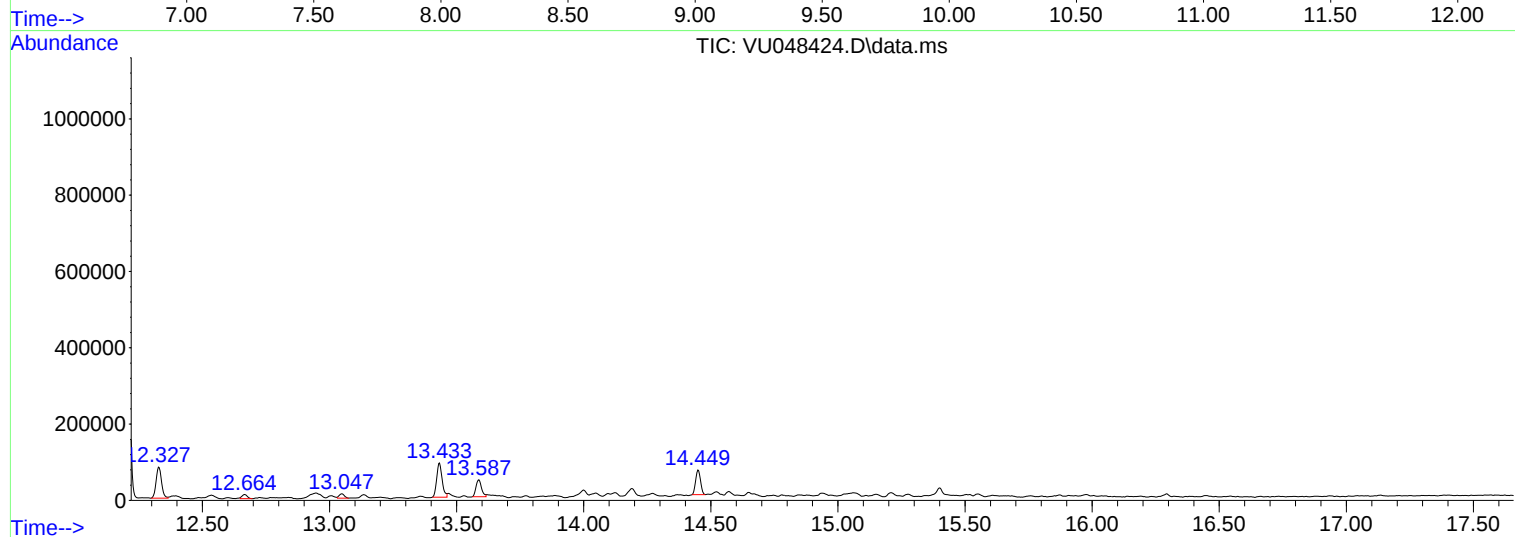
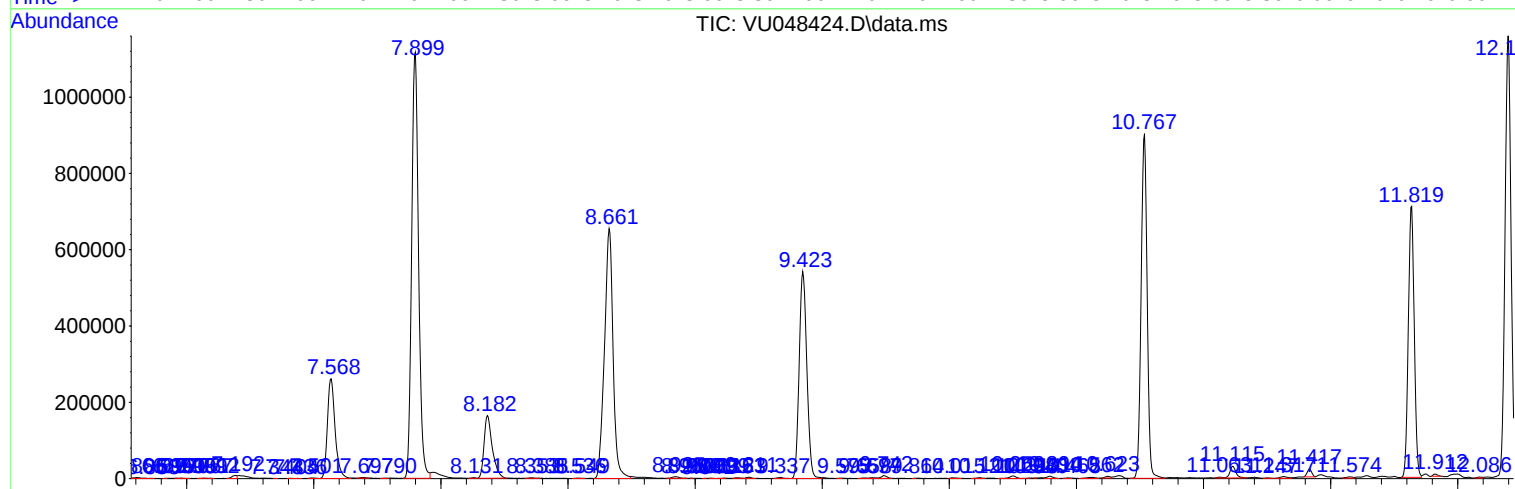
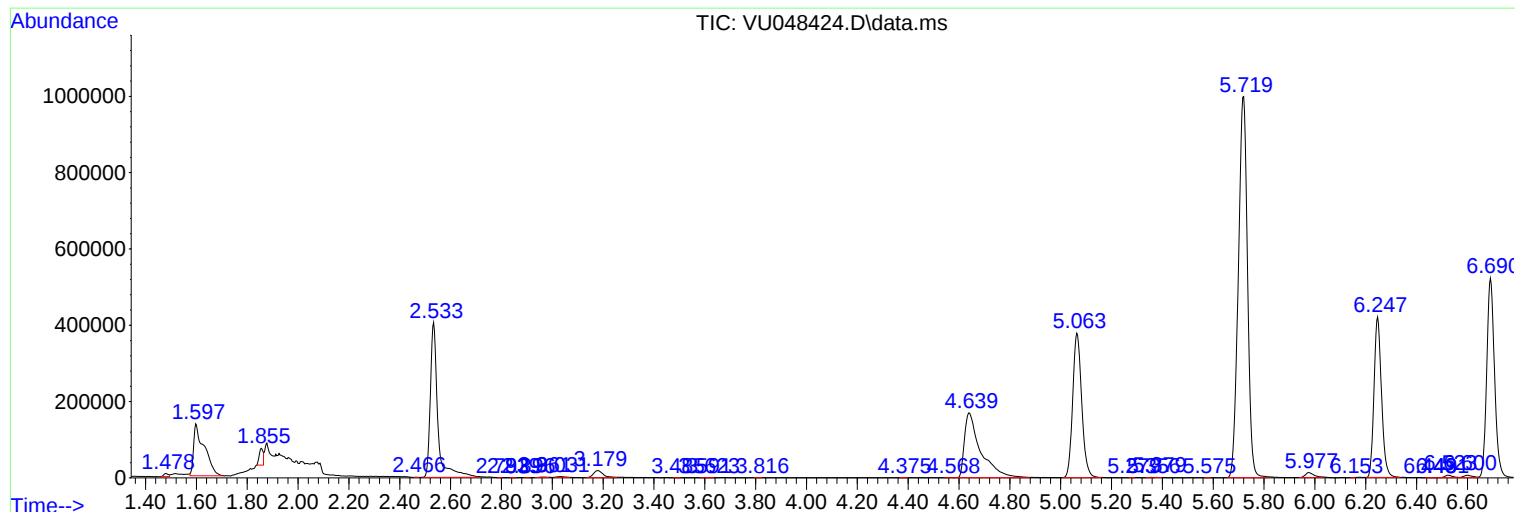
Sum of corrected areas: 18380388

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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4B6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4B6ME

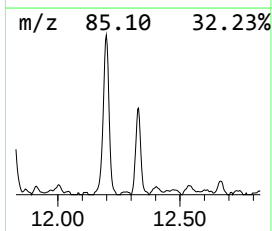
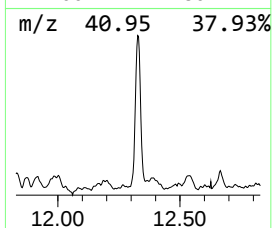
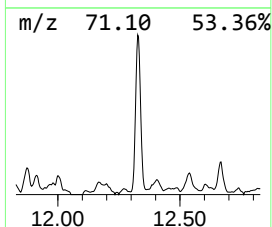
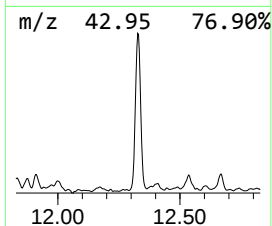
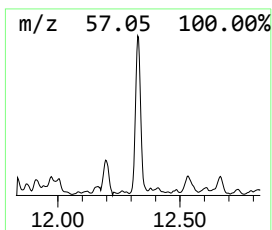
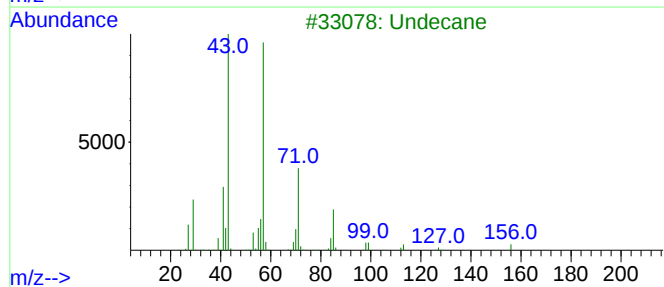
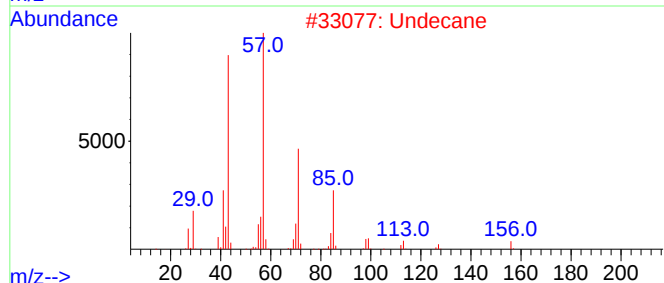
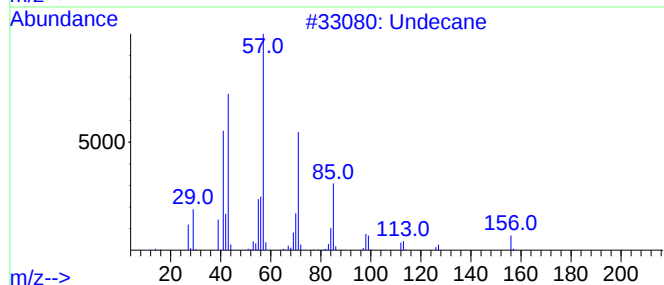
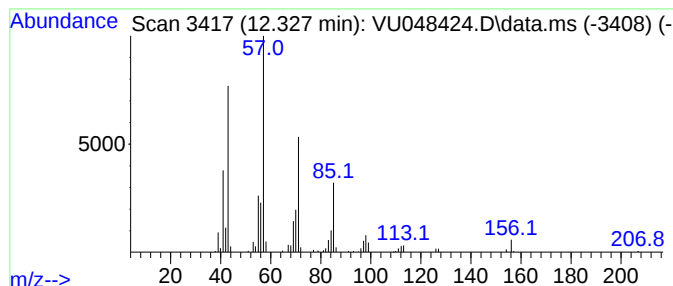
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.327	5.27 ug/L	119967	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	81
2	Undecane			156	C11H24	001120-21-4	72
3	Undecane			156	C11H24	001120-21-4	68
4	Nonane			128	C9H20	000111-84-2	64
5	Undecane			156	C11H24	001120-21-4	62



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Misc : 7.49g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4B6ME

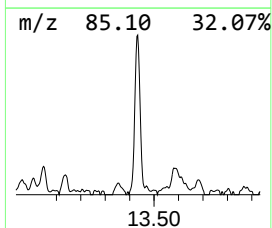
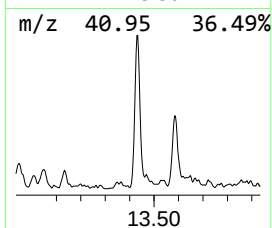
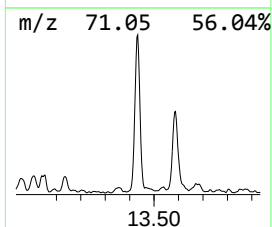
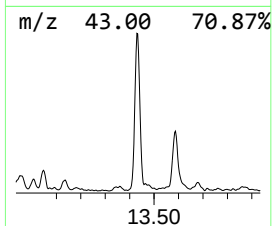
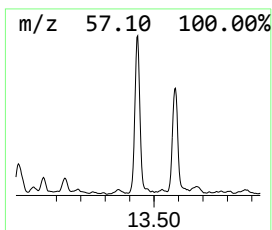
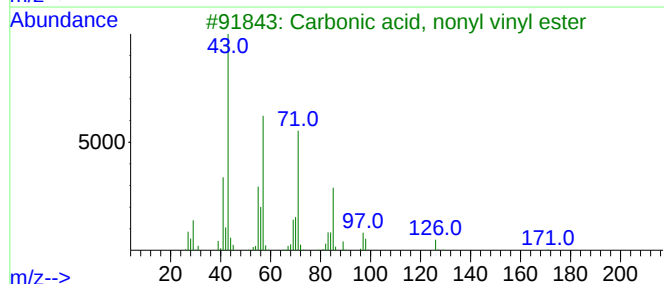
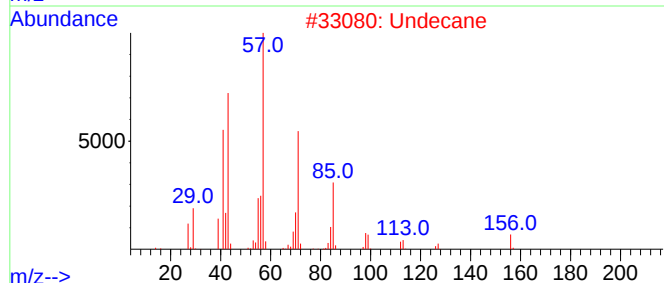
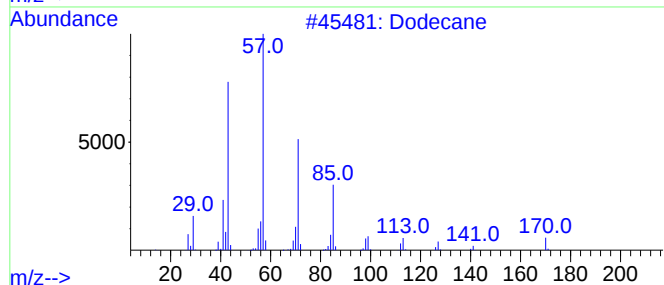
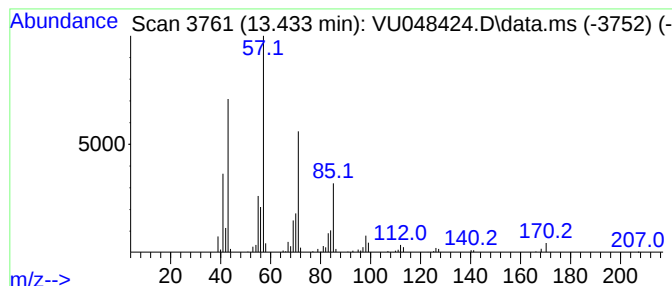
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.433	5.87 ug/L	133725	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	83
2			Undecane	156	C11H24	001120-21-4	78
3			Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	64
4			Ether, hexyl pentyl	172	C11H24O	032357-83-8	58
5			Dodecane	170	C12H26	000112-40-3	58



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Instrument :
MSVOA_U
ClientSampleId :
EW4B6ME

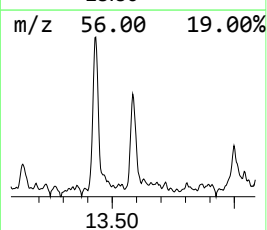
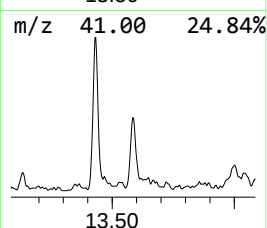
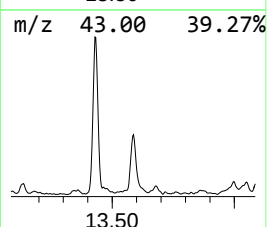
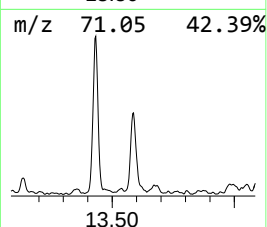
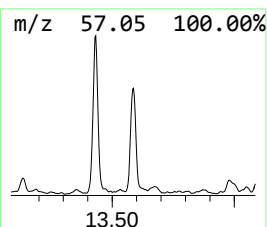
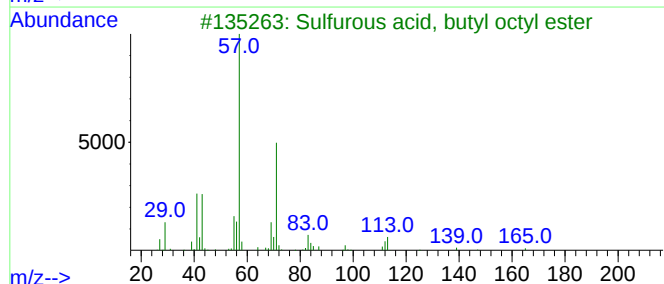
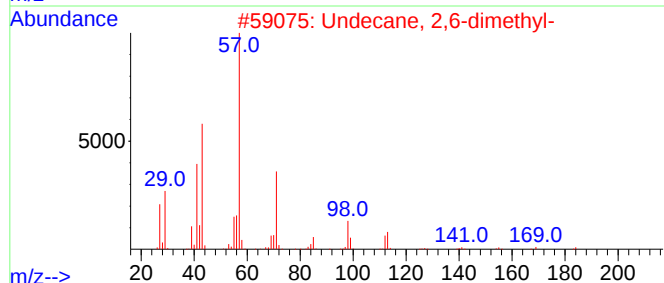
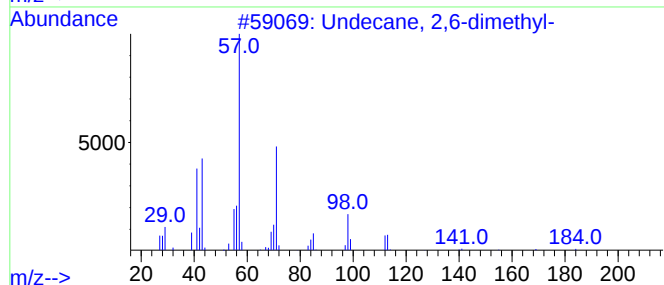
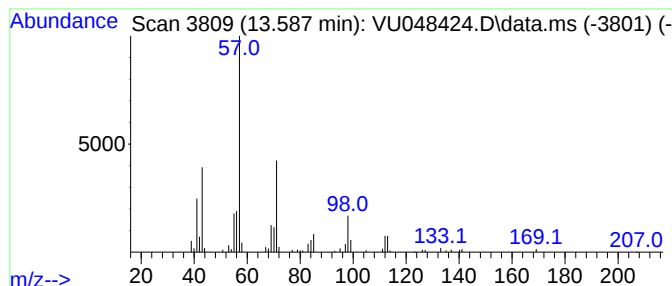
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.587	2.98 ug/L	67922	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	90
2	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	83
3	Sulfurous acid, butyl octyl ester	250	C12H26O3S	1000309-17-5	72
4	5-Ethyldecane	170	C12H26	017302-36-2	72
5	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050422\
Data File : VU048424.D
Acq On : 04 May 2022 19:43
Operator : SY/MD
Sample : N2632-14ME
Misc : 7.49g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4B6ME

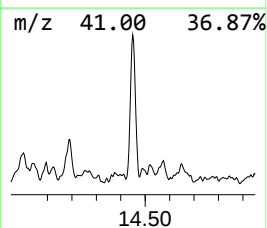
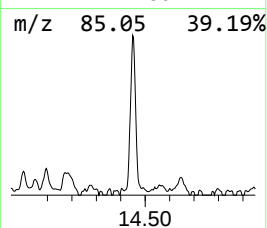
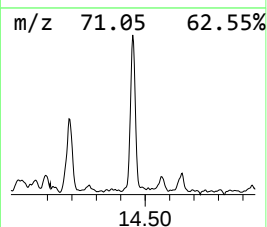
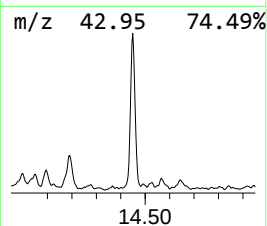
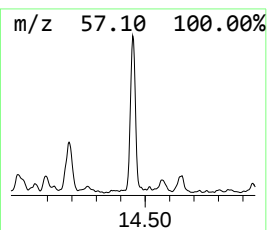
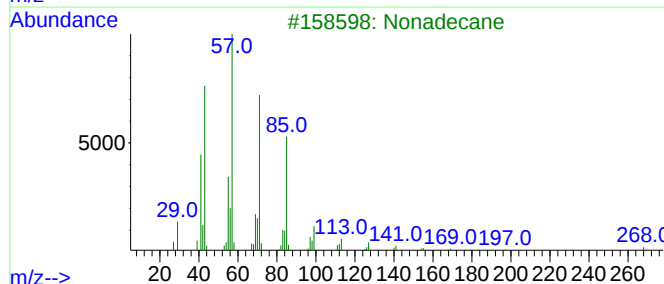
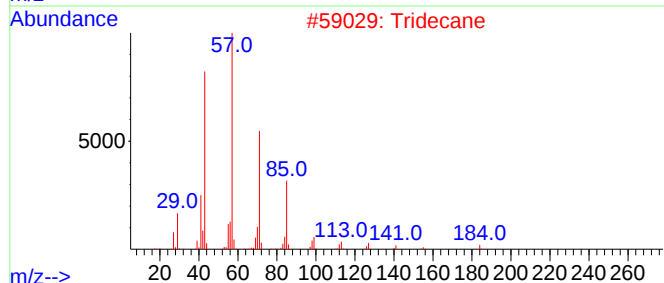
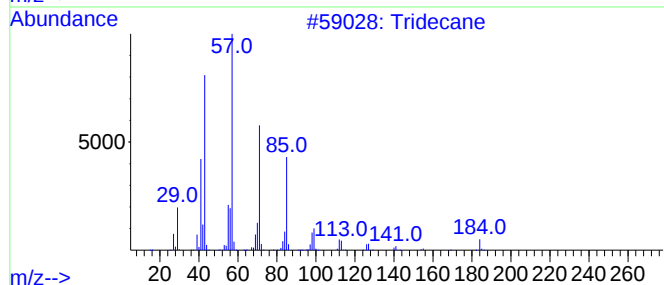
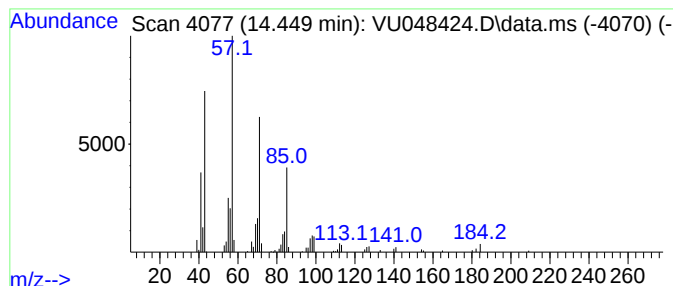
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Quant Title : VOC Analysis

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.449	3.73 ug/L	85058	1,4-Dichlorobenzene-d4	11.819

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecane	184	C13H28	000629-50-5	97
2		Tridecane	184	C13H28	000629-50-5	93
3		Nonadecane	268	C19H40	000629-92-5	91
4		Dodecane	170	C12H26	000112-40-3	90
5		Tridecane	184	C13H28	000629-50-5	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050422\
Data File : VU048424.D
Acq On : 04 May 2022 19:43
Operator : SY/MD
Sample : N2632-14ME
Misc : 7.49g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4B6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

					--Internal Standard--				
TIC Top	Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL)	Alkane: S...	12.327	5.3	ug/L	119967	3	11.819	1138990	50.0
(DEL)	Alkane: S...	13.433	5.9	ug/L	133725	3	11.819	1138990	50.0
(DEL)	Alkane: S...	13.587	3.0	ug/L	67922	3	11.819	1138990	50.0
(DEL)	Alkane: S...	14.449	3.7	ug/L	85058	3	11.819	1138990	50.0