

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033123\
 Data File : VU053506.D
 Acq On : 31 Mar 2023 20:55
 Operator : JC/MD
 Sample : 02121-15ME
 Misc : 3.42g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C1188ME

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\SFAMULM033123WMA.M

Title : VOC Analysis

Signal : TIC: VU053506.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.459	30	37	42	rBV3	4897	8029	0.59%	0.060%
2	1.597	71	80	102	rBV	141157	209194	15.43%	1.553%
3	1.871	161	165	182	rVB	41921	55651	4.10%	0.413%
4	2.539	360	373	393	rVV	302360	492400	36.31%	3.655%
5	2.629	394	401	417	rVB3	2484	5061	0.37%	0.038%
6	2.700	420	423	427	rBV2	641	527	0.04%	0.004%
7	2.761	440	442	444	rBV2	414	260	0.02%	0.002%
8	2.813	455	458	460	rBV2	321	248	0.02%	0.002%
9	2.861	470	473	475	rBV2	460	264	0.02%	0.002%
10	2.948	491	500	511	rBV3	1929	3240	0.24%	0.024%
11	3.028	514	525	526	rBV5	5039	6131	0.45%	0.046%
12	3.099	544	547	549	rBV2	484	284	0.02%	0.002%
13	3.166	562	568	569	rBV2	1000	806	0.06%	0.006%
14	3.256	590	596	597	rBV2	277	254	0.02%	0.002%
15	3.337	609	621	631	rVB7	5303	10493	0.77%	0.078%
16	3.378	631	634	637	rBV	417	389	0.03%	0.003%
17	3.549	680	687	689	rBV4	305	252	0.02%	0.002%
18	3.562	689	691	693	rVV	486	245	0.02%	0.002%
19	3.674	715	726	739	rVV6	3478	7519	0.55%	0.056%
20	3.854	770	782	796	rBV3	3070	6638	0.49%	0.049%
21	4.240	899	902	906	rVV2	261	249	0.02%	0.002%
22	4.272	906	912	916	rVV2	1326	1589	0.12%	0.012%
23	4.411	946	955	956	rBV2	567	616	0.05%	0.005%
24	4.494	975	981	982	rBV	998	713	0.05%	0.005%
25	4.510	982	986	989	rBV2	806	727	0.05%	0.005%
26	4.626	1008	1022	1058	rBV3	77885	285899	21.08%	2.122%
27	4.867	1095	1097	1101	rVB3	558	316	0.02%	0.002%
28	4.989	1128	1135	1138	rBV2	281	257	0.02%	0.002%
29	5.054	1138	1155	1185	rBV	224734	526192	38.80%	3.905%
30	5.301	1220	1232	1243	rBV3	15842	36943	2.72%	0.274%
31	5.578	1307	1318	1328	rBV4	5041	10412	0.77%	0.077%
32	5.713	1340	1360	1391	rBV2	490350	1281607	94.51%	9.512%
33	5.829	1393	1396	1406	rVB5	1965	3012	0.22%	0.022%
34	5.915	1416	1423	1430	rVB6	777	1310	0.10%	0.010%
35	5.970	1430	1440	1452	rBV7	3446	7832	0.58%	0.058%
36	6.028	1457	1458	1464	rVB3	774	567	0.04%	0.004%

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Integration Parameters: LSCINT.P

Integrator: RTE

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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\SFAMULM033123WMA.M
 Title : VOC Analysis

37	6.121	1474	1487	1502	rBV6	8432	16610	1.22%	0.123%
38	6.240	1509	1524	1549	rBV	434955	841192	62.03%	6.243%
39	6.533	1601	1615	1629	rBV4	73724	145055	10.70%	1.077%
40	6.684	1647	1662	1675	rBV	278194	561578	41.41%	4.168%
41	6.751	1676	1683	1708	rVV3	42640	87751	6.47%	0.651%
42	6.854	1708	1715	1728	rVB5	2626	4366	0.32%	0.032%
43	6.970	1746	1751	1761	rVB5	1394	2245	0.17%	0.017%
44	7.057	1767	1778	1786	rBV6	2624	5272	0.39%	0.039%
45	7.198	1815	1822	1825	rBV5	1742	2042	0.15%	0.015%
46	7.330	1854	1863	1869	rBV4	1023	1482	0.11%	0.011%
47	7.407	1876	1887	1888	rBV3	1773	1938	0.14%	0.014%
48	7.491	1901	1913	1920	rBV4	7149	12458	0.92%	0.092%
49	7.562	1921	1935	1953	rVV	161681	307292	22.66%	2.281%
50	7.648	1956	1962	1970	rVV6	4899	7356	0.54%	0.055%
51	7.738	1987	1990	1992	rBV2	686	343	0.03%	0.003%
52	7.758	1992	1996	2003	rVB3	962	848	0.06%	0.006%
53	7.848	2009	2024	2026	rBV3	17123	24962	1.84%	0.185%
54	7.893	2027	2038	2055	rVB	637470	1130661	83.38%	8.392%
55	8.124	2102	2110	2116	rBV3	16730	24212	1.79%	0.180%
56	8.176	2116	2126	2139	rBV	102847	189502	13.97%	1.406%
57	8.362	2174	2184	2197	rVB5	6167	11150	0.82%	0.083%
58	8.430	2197	2205	2207	rBV6	1673	2053	0.15%	0.015%
59	8.545	2229	2241	2251	rVB6	8946	17450	1.29%	0.130%
60	8.642	2255	2271	2298	rBV2	305087	608030	44.84%	4.513%
61	8.754	2300	2306	2313	rBV3	3200	4280	0.32%	0.032%
62	8.857	2331	2338	2347	rVB2	12386	19056	1.41%	0.141%
63	8.918	2347	2357	2366	rBV3	15052	25852	1.91%	0.192%
64	9.037	2389	2394	2395	rBV4	718	549	0.04%	0.004%
65	9.057	2395	2400	2403	rVV5	1205	1387	0.10%	0.010%
66	9.115	2411	2418	2424	rBV4	4915	7226	0.53%	0.054%
67	9.163	2426	2433	2439	rVV7	6001	10825	0.80%	0.080%
68	9.208	2440	2447	2459	rVB2	13958	22249	1.64%	0.165%
69	9.330	2471	2485	2496	rBV2	10201	17447	1.29%	0.129%
70	9.417	2498	2512	2531	rBV	578793	1036068	76.40%	7.690%
71	9.565	2548	2558	2567	rBV	7411	12618	0.93%	0.094%
72	9.693	2578	2598	2606	rBV3	38040	84986	6.27%	0.631%
73	9.738	2607	2612	2637	rVB	42941	74000	5.46%	0.549%
74	9.886	2643	2658	2667	rBV	2331	5468	0.40%	0.041%
75	9.944	2671	2676	2678	rBV3	1288	1091	0.08%	0.008%
76	10.012	2687	2697	2706	rBV7	9718	22878	1.69%	0.170%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
 Title : VOC Analysis

77	10.105	2719	2726	2739	rVB5	21967	41684	3.07%	0.309%
78	10.246	2753	2770	2783	rBV7	15197	38190	2.82%	0.283%
79	10.352	2794	2803	2811	rBV5	16712	28687	2.12%	0.213%
80	10.449	2831	2833	2836	rBV2	866	640	0.05%	0.005%
81	10.481	2837	2843	2851	rVB3	3751	5844	0.43%	0.043%
82	10.697	2903	2910	2915	rBV9	3901	5760	0.42%	0.043%
83	10.754	2915	2928	2940	rBV	468791	756804	55.81%	5.617%
84	10.906	2965	2975	2982	rBV	13236	20978	1.55%	0.156%
85	10.999	2996	3004	3008	rBV3	24298	38488	2.84%	0.286%
86	11.227	3073	3075	3077	rBV2	835	501	0.04%	0.004%
87	11.298	3087	3097	3110	rBV4	13605	34356	2.53%	0.255%
88	11.410	3126	3132	3140	rVB2	24954	33875	2.50%	0.251%
89	11.465	3140	3149	3173	rVB2	52948	103769	7.65%	0.770%
90	11.809	3244	3256	3270	rBV	794734	1265319	93.31%	9.391%
91	11.999	3310	3315	3322	rVB6	13522	16242	1.20%	0.121%
92	12.121	3337	3353	3361	rBV4	23278	55466	4.09%	0.412%
93	12.192	3362	3375	3394	rVV	808161	1356066	100.00%	10.065%
94	12.323	3407	3416	3425	rVB	166984	232881	17.17%	1.728%
95	13.426	3750	3759	3780	rVB	244321	389490	28.72%	2.891%
96	13.581	3803	3807	3816	rVB3	27237	32882	2.42%	0.244%
97	14.446	4068	4076	4087	rBV	207297	281567	20.76%	2.090%
98	15.217	4308	4316	4326	rVB2	87452	139612	10.30%	1.036%
99	15.397	4365	4372	4397	rVB4	118881	238060	17.56%	1.767%
100	16.404	4681	4685	4691	rVB3	35318	38479	2.84%	0.286%

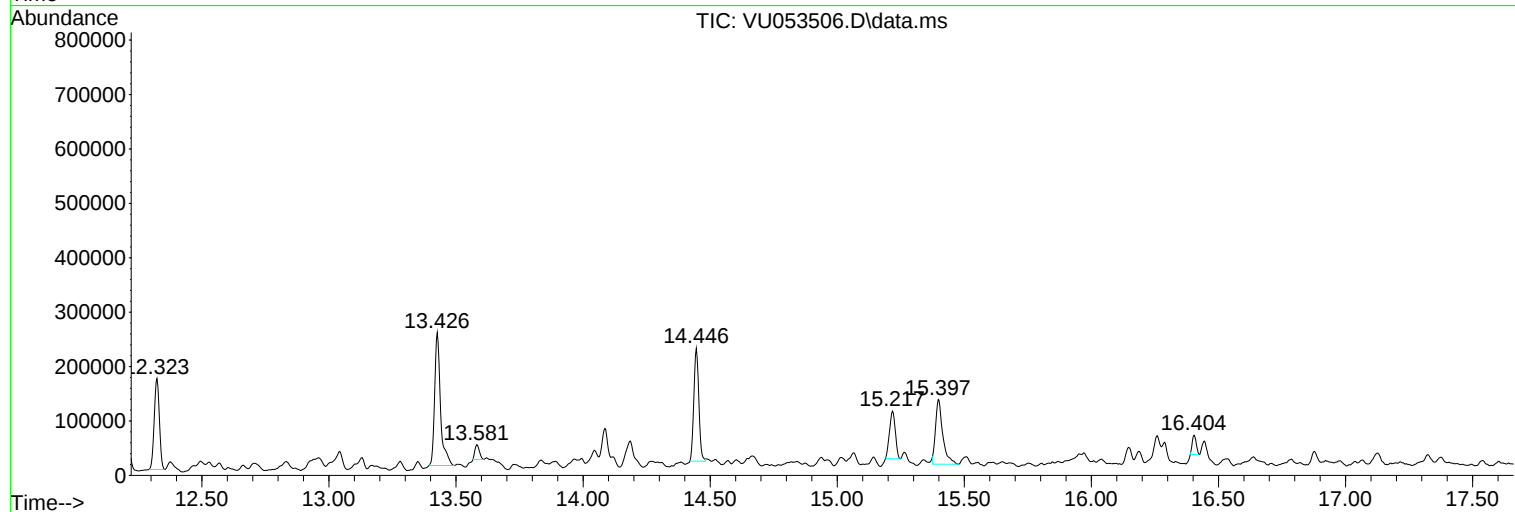
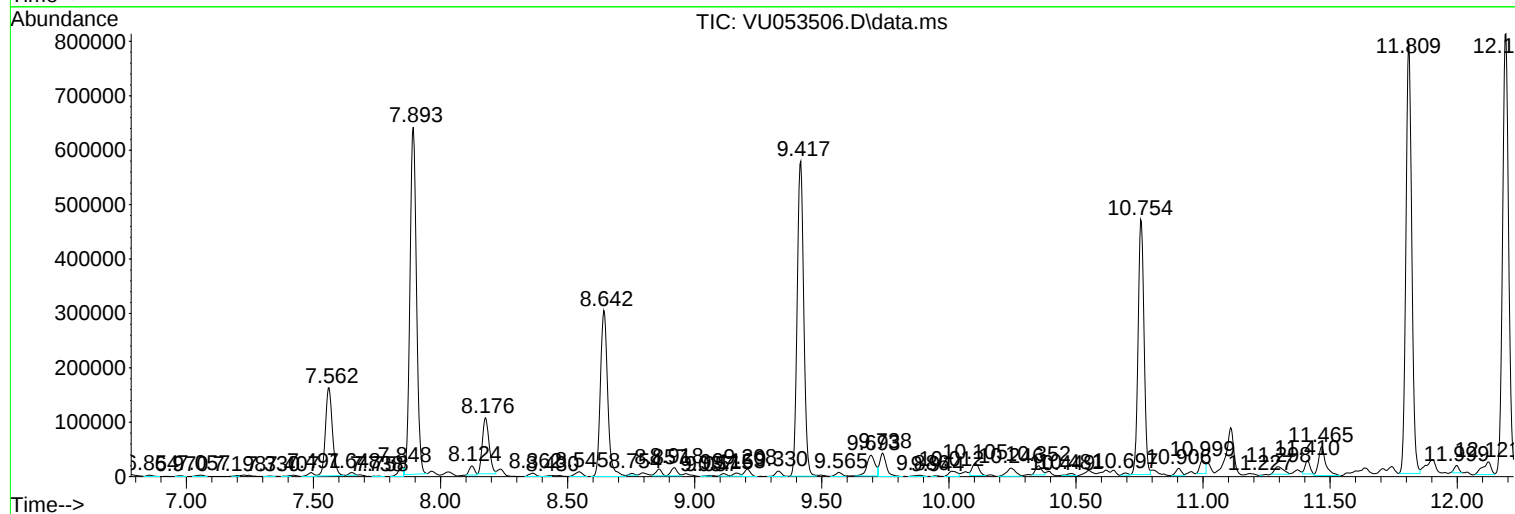
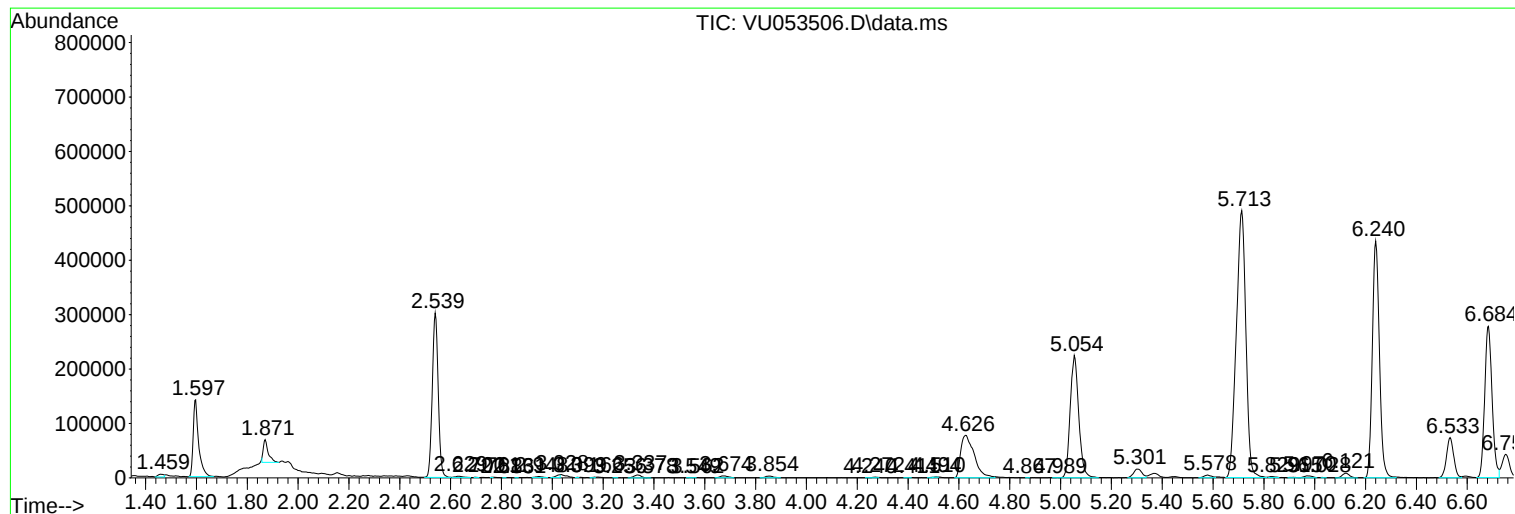
Sum of corrected areas: 13473594

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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C1188ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.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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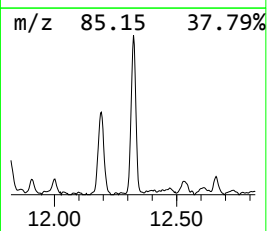
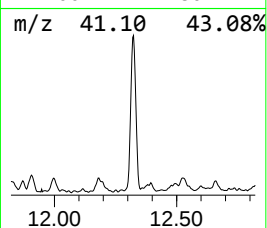
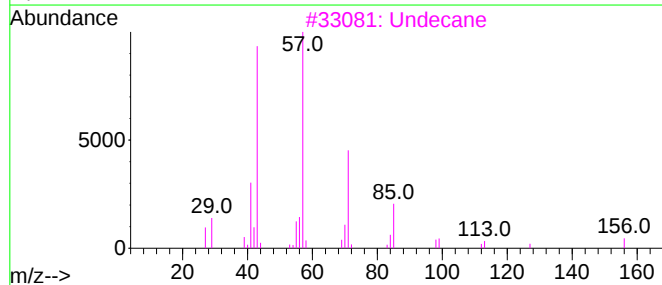
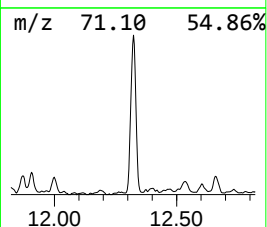
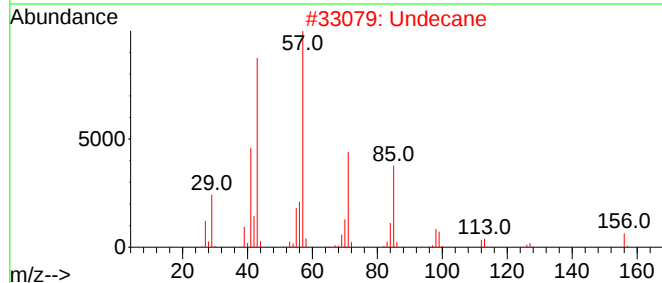
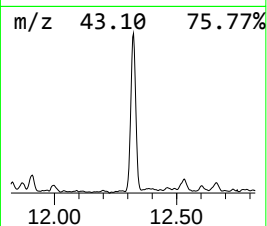
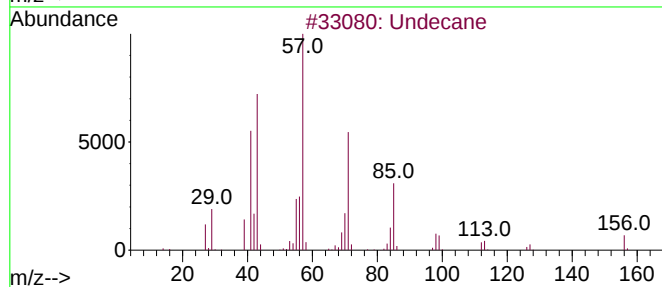
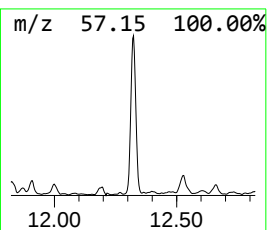
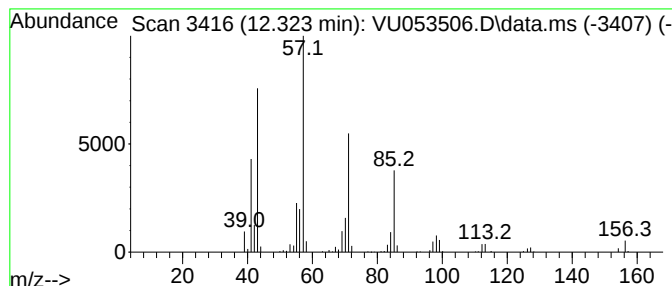
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.323	9.20 ug/L	232881	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	95
2	Undecane			156	C11H24	001120-21-4	93
3	Undecane			156	C11H24	001120-21-4	91
4	Undecane			156	C11H24	001120-21-4	91
5	Undecane			156	C11H24	001120-21-4	90



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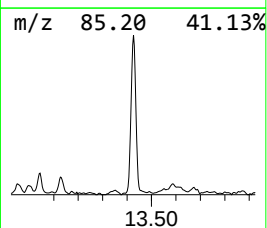
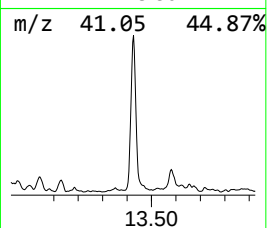
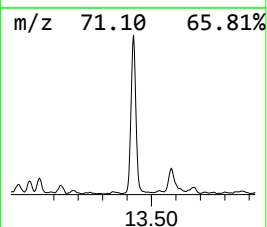
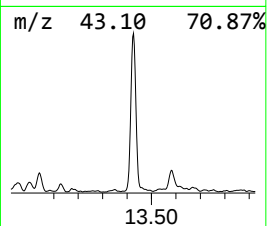
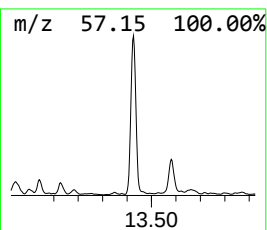
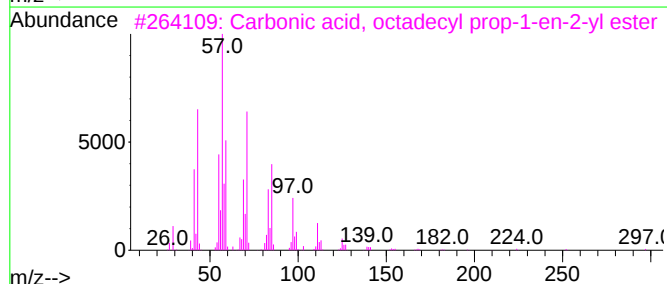
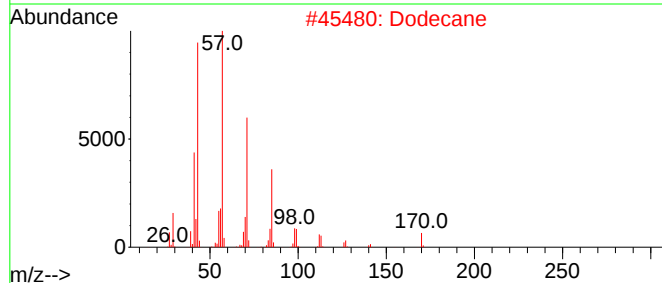
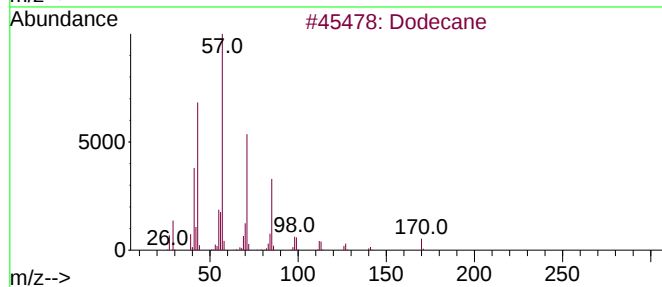
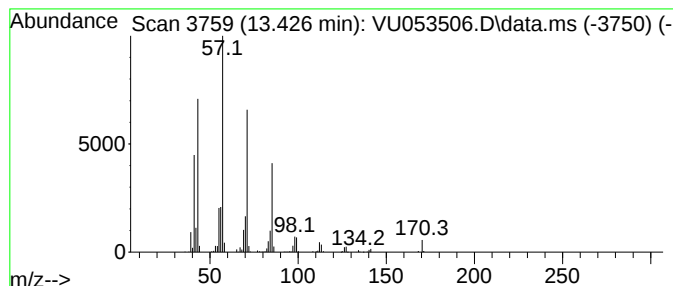
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.426	15.39 ug/L	389490	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	97
2			Dodecane	170	C12H26	000112-40-3	93
3			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	90
4			Tetradecane	198	C14H30	000629-59-4	90
5			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	83



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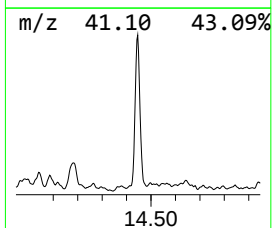
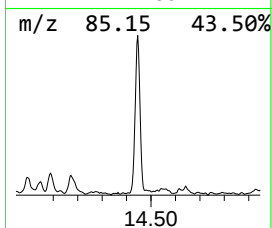
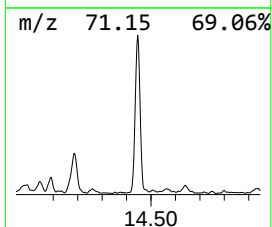
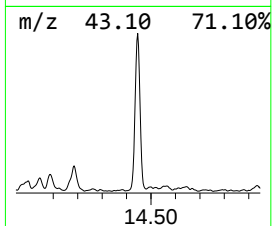
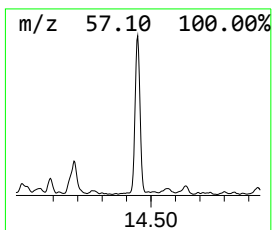
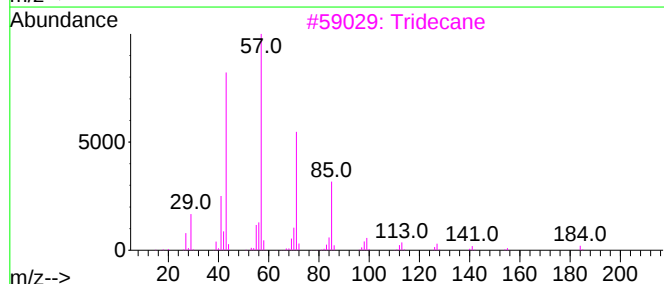
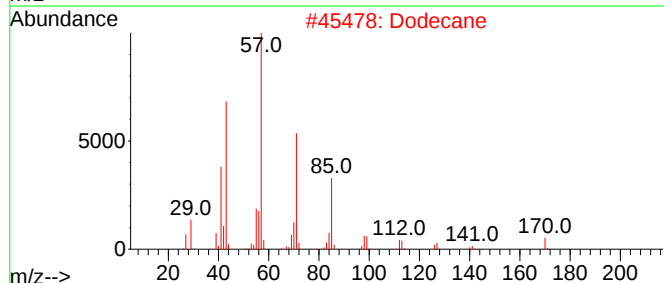
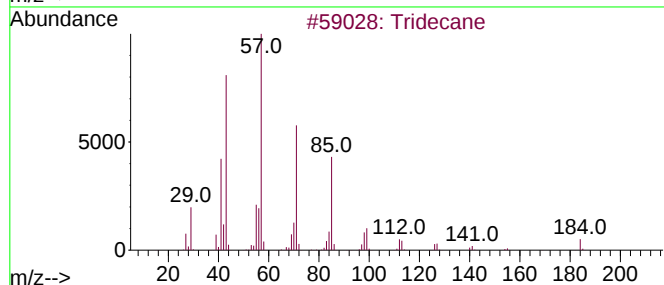
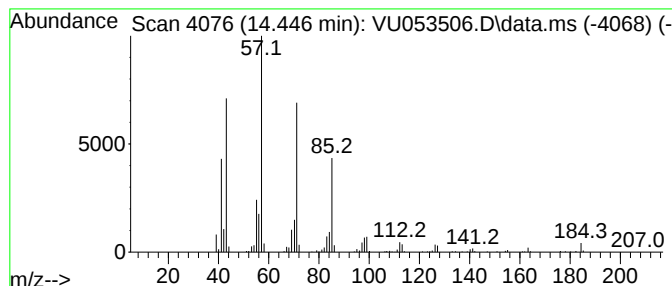
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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.
14.446	11.13 ug/L	281567	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	96
2			Dodecane	170	C12H26	000112-40-3	90
3			Tridecane	184	C13H28	000629-50-5	87
4			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	86
5			Tetradecane	198	C14H30	000629-59-4	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033123\
Data File : VU053506.D
Acq On : 31 Mar 2023 20:55
Operator : JC/MD
Sample : 02121-15ME
Misc : 3.42g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C1188ME

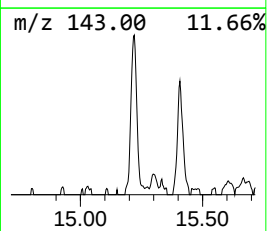
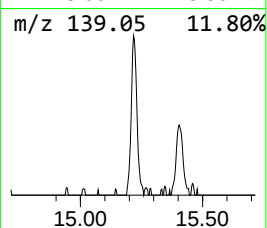
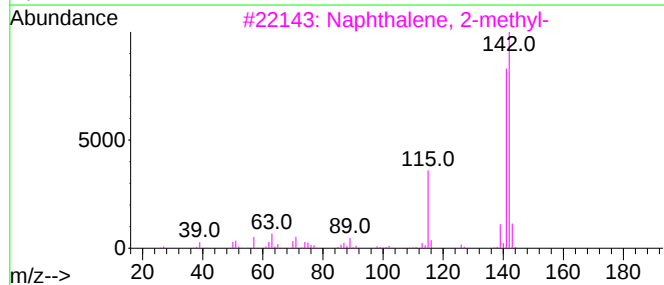
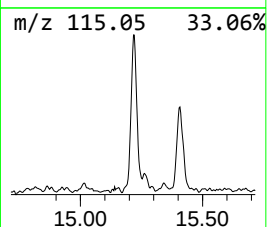
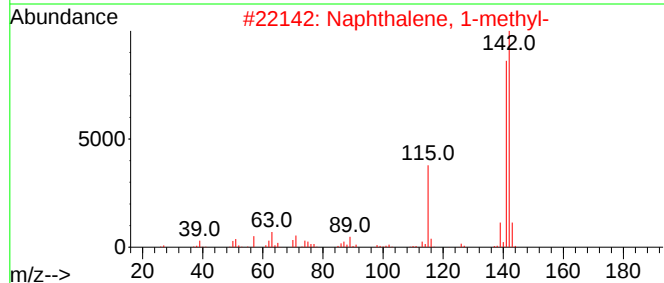
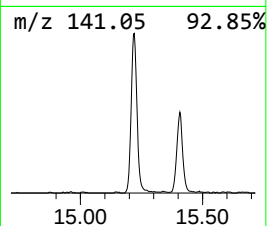
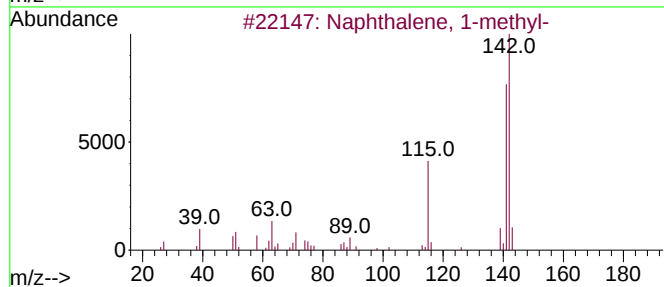
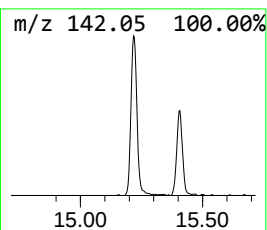
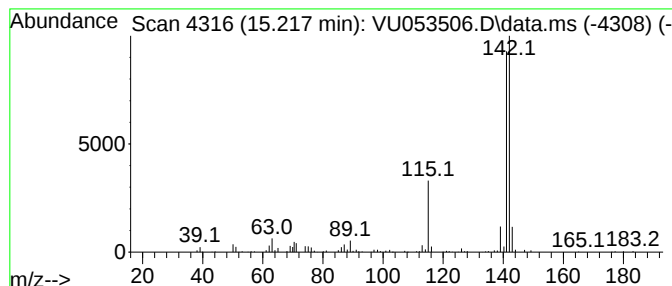
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Quant Title : VOC Analysis

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

Peak Number 5 Naphthalene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.217	5.52 ug/L	139612	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
3			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	94
4			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	94
5			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033123\
Data File : VU053506.D
Acq On : 31 Mar 2023 20:55
Operator : JC/MD
Sample : 02121-15ME
Misc : 3.42g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C1188ME

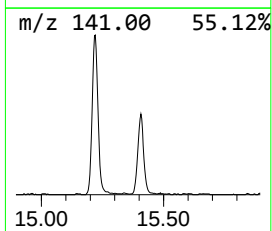
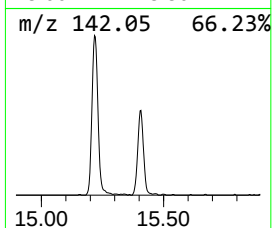
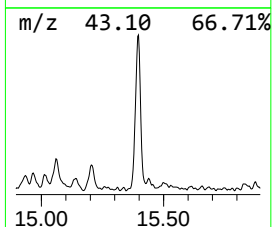
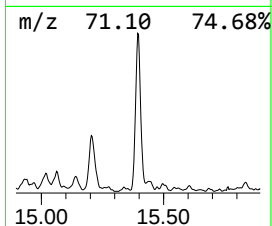
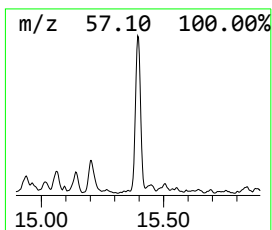
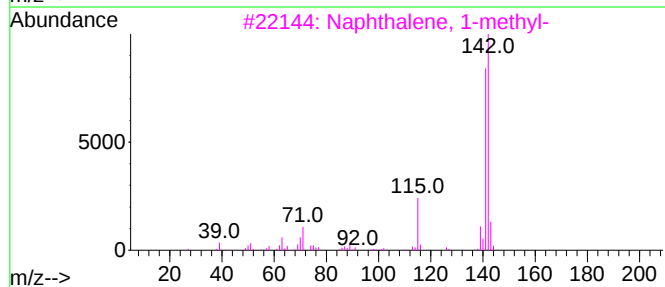
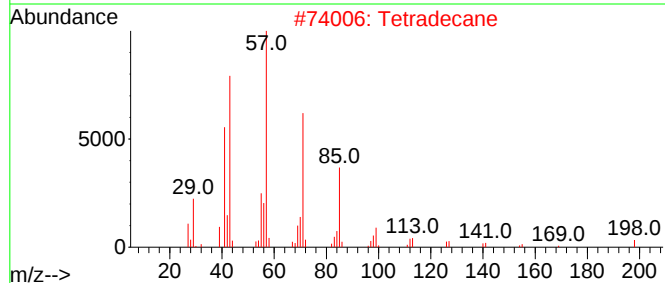
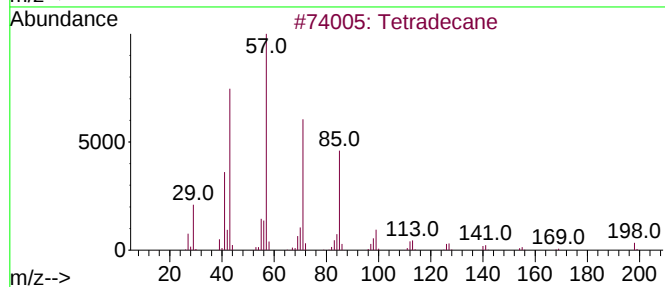
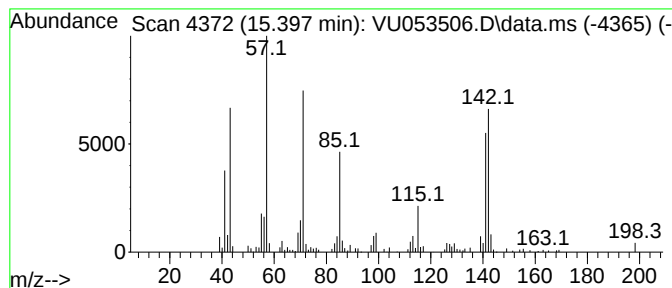
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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.
15.397	9.41 ug/L	238060	1,4-Dichlorobenzene-d4	11.809

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane	198	C14H30	000629-59-4	95
2		Tetradecane	198	C14H30	000629-59-4	87
3		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	68
4		1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	62
5		Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033123\
Data File : VU053506.D
Acq On : 31 Mar 2023 20:55
Operator : JC/MD
Sample : 02121-15ME
Misc : 3.42g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C1188ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.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...	12.323	9.2	ug/L	232881	3	11.809	1265320	50.0
(DEL) Alkane: S...	13.426	15.4	ug/L	389490	3	11.809	1265320	50.0
(DEL) Alkane: S...	14.446	11.1	ug/L	281567	3	11.809	1265320	50.0
Naphthalene, 1-...	15.217	5.5	ug/L	139612	3	11.809	1265320	50.0
(DEL) Alkane: S...	15.397	9.4	ug/L	238060	3	11.809	1265320	50.0