

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040323\
 Data File : VU053513.D
 Acq On : 03 Apr 2023 12:30
 Operator : JC/MD
 Sample : 02121-15ME
 Misc : 3.42g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 6 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: VU053513.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	95	rBV	73934	97664	10.30%	1.005%
2	1.774	123	135	136	rBV8	11412	16775	1.77%	0.173%
3	1.874	161	166	189	rVB3	59591	130517	13.77%	1.344%
4	2.546	364	375	393	rVB	155032	255476	26.96%	2.630%
5	2.626	393	400	405	rBV3	1878	2567	0.27%	0.026%
6	2.768	441	444	448	rBV2	561	536	0.06%	0.006%
7	2.948	490	500	509	rBV3	2199	3622	0.38%	0.037%
8	3.038	518	528	540	rVV4	4008	8826	0.93%	0.091%
9	3.173	563	570	572	rBV2	676	778	0.08%	0.008%
10	3.340	611	622	633	rBV7	2619	4910	0.52%	0.051%
11	3.678	718	727	728	rBV4	1209	1285	0.14%	0.013%
12	3.854	771	782	798	rVV3	2091	4951	0.52%	0.051%
13	4.269	907	911	918	rBV2	510	696	0.07%	0.007%
14	4.514	979	987	993	rVV3	868	1479	0.16%	0.015%
15	4.620	1008	1020	1060	rBV2	51055	192874	20.35%	1.986%
16	5.054	1139	1155	1176	rBV2	141367	322496	34.03%	3.320%
17	5.304	1216	1233	1244	rBV2	15222	33380	3.52%	0.344%
18	5.372	1246	1254	1266	rVV6	5207	12177	1.28%	0.125%
19	5.446	1269	1277	1288	rVB5	1458	2824	0.30%	0.029%
20	5.578	1312	1318	1327	rBV7	2293	4211	0.44%	0.043%
21	5.629	1332	1334	1340	rVB4	1357	1029	0.11%	0.011%
22	5.716	1340	1361	1390	rBV2	286999	770386	81.29%	7.931%
23	5.838	1395	1399	1409	rVV7	1599	2326	0.25%	0.024%
24	5.912	1416	1422	1426	rBV4	915	917	0.10%	0.009%
25	5.976	1431	1442	1457	rBV6	2774	6130	0.65%	0.063%
26	6.124	1479	1488	1498	rVV4	4977	9285	0.98%	0.096%
27	6.240	1509	1524	1545	rBV	316604	614619	64.85%	6.328%
28	6.533	1599	1615	1629	rBV5	52434	105104	11.09%	1.082%
29	6.684	1648	1662	1675	rBV	173775	347424	36.66%	3.577%
30	6.755	1676	1684	1706	rVB4	32581	67195	7.09%	0.692%
31	6.854	1709	1715	1716	rBV3	1321	1217	0.13%	0.013%
32	6.973	1749	1752	1757	rVB4	947	812	0.09%	0.008%
33	7.054	1768	1777	1788	rVB5	1952	3750	0.40%	0.039%
34	7.192	1811	1820	1821	rVV2	1630	1699	0.18%	0.017%
35	7.221	1824	1829	1838	rVB6	1597	2840	0.30%	0.029%
36	7.324	1859	1861	1869	rVB3	754	942	0.10%	0.010%

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Integration Parameters: LSCINT.P

Integrator: RTE

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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\SFAMULM033123WMA.M
 Title : VOC Analysis

37	7.414	1883	1889	1900	rVB5	2377	3855	0.41%	0.040%
38	7.491	1900	1913	1920	rBV4	5158	9661	1.02%	0.099%
39	7.562	1922	1935	1949	rVB	100098	182958	19.30%	1.884%
40	7.652	1957	1963	1970	rBV6	3867	5237	0.55%	0.054%
41	7.748	1987	1993	1997	rBV3	518	526	0.06%	0.005%
42	7.806	2006	2011	2012	rBV2	762	496	0.05%	0.005%
43	7.848	2013	2024	2026	rVV4	13417	18993	2.00%	0.196%
44	7.893	2028	2038	2055	rVV	381008	662625	69.92%	6.822%
45	7.964	2055	2060	2069	rVV3	7626	14451	1.52%	0.149%
46	8.028	2072	2080	2092	rVB4	6870	13833	1.46%	0.142%
47	8.124	2101	2110	2117	rBV2	12308	19709	2.08%	0.203%
48	8.176	2117	2126	2138	rVV	70508	125921	13.29%	1.296%
49	8.237	2140	2145	2155	rVV4	11642	18414	1.94%	0.190%
50	8.359	2171	2183	2197	rBV6	5192	9637	1.02%	0.099%
51	8.423	2197	2203	2204	rBV4	1344	1169	0.12%	0.012%
52	8.536	2227	2238	2240	rBV6	3258	4832	0.51%	0.050%
53	8.639	2255	2270	2295	rBV2	208993	397418	41.93%	4.092%
54	8.755	2299	2306	2312	rBV6	3515	5047	0.53%	0.052%
55	8.861	2331	2339	2347	rVB4	10924	18066	1.91%	0.186%
56	8.918	2347	2357	2365	rBV4	13633	23249	2.45%	0.239%
57	9.060	2395	2401	2410	rVV7	1754	2642	0.28%	0.027%
58	9.115	2410	2418	2425	rVV5	4966	8044	0.85%	0.083%
59	9.166	2425	2434	2440	rVV5	6094	11491	1.21%	0.118%
60	9.208	2441	2447	2458	rVB4	11444	18732	1.98%	0.193%
61	9.330	2476	2485	2495	rBV2	9515	14571	1.54%	0.150%
62	9.414	2495	2511	2530	rBV	464039	795537	83.94%	8.190%
63	9.568	2548	2559	2567	rBV	7156	11778	1.24%	0.121%
64	9.690	2580	2597	2606	rVV	38471	82491	8.70%	0.849%
65	9.738	2607	2612	2632	rVB3	35912	60001	6.33%	0.618%
66	9.883	2649	2657	2666	rVB8	2350	4048	0.43%	0.042%
67	9.947	2671	2677	2682	rBV5	963	1485	0.16%	0.015%
68	10.018	2688	2699	2707	rBV5	8721	20216	2.13%	0.208%
69	10.102	2718	2725	2740	rVB3	20493	41935	4.42%	0.432%
70	10.243	2754	2769	2770	rBV6	14107	19894	2.10%	0.205%
71	10.317	2784	2792	2794	rBV7	2081	2912	0.31%	0.030%
72	10.356	2794	2804	2811	rBV6	15525	27959	2.95%	0.288%
73	10.436	2824	2829	2830	rBV2	1534	1003	0.11%	0.010%
74	10.552	2852	2865	2872	rBV9	9016	18914	2.00%	0.195%
75	10.690	2904	2908	2910	rBV5	2849	2331	0.25%	0.024%
76	10.754	2916	2928	2940	rBV	317520	509450	53.75%	5.245%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Stop Thrs : 0

Peak Location: TOP

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

77	10.906	2964	2975	2982	rBV3	12082	20383	2.15%	0.210%
78	10.951	2984	2989	2995	rBV6	4724	5027	0.53%	0.052%
79	10.999	2996	3004	3008	rBV2	23427	37699	3.98%	0.388%
80	11.108	3027	3038	3051	rVB3	76609	150507	15.88%	1.550%
81	11.237	3074	3078	3084	rBV5	1852	2475	0.26%	0.025%
82	11.291	3088	3095	3109	rVV4	13031	26623	2.81%	0.274%
83	11.372	3114	3120	3124	rVV5	7723	11117	1.17%	0.114%
84	11.414	3126	3133	3140	rVV3	24775	34976	3.69%	0.360%
85	11.465	3141	3149	3171	rVB	51684	94963	10.02%	0.978%
86	11.574	3174	3183	3187	rBV8	4415	8032	0.85%	0.083%
87	11.703	3219	3223	3225	rBV3	5881	5257	0.55%	0.054%
88	11.809	3244	3256	3270	rBV	595304	947750	100.00%	9.757%
89	11.999	3309	3315	3323	rVB4	12319	17250	1.82%	0.178%
90	12.121	3337	3353	3362	rBV4	26146	57374	6.05%	0.591%
91	12.188	3362	3374	3392	rVV	516536	868002	91.59%	8.936%
92	12.324	3407	3416	3425	rBV	148073	202752	21.39%	2.087%
93	13.349	3729	3735	3744	rBV3	13624	20915	2.21%	0.215%
94	13.426	3750	3759	3778	rVB	218469	342476	36.14%	3.526%
95	13.584	3803	3808	3816	rBV3	24857	29587	3.12%	0.305%
96	14.446	4068	4076	4093	rBV	160972	230792	24.35%	2.376%
97	15.217	4309	4316	4325	rVB	76463	115620	12.20%	1.190%
98	15.401	4365	4373	4397	rVB4	79310	170138	17.95%	1.752%
99	16.147	4600	4605	4612	rBV5	21873	27664	2.92%	0.285%
100	16.407	4678	4686	4691	rBV	39260	60415	6.37%	0.622%

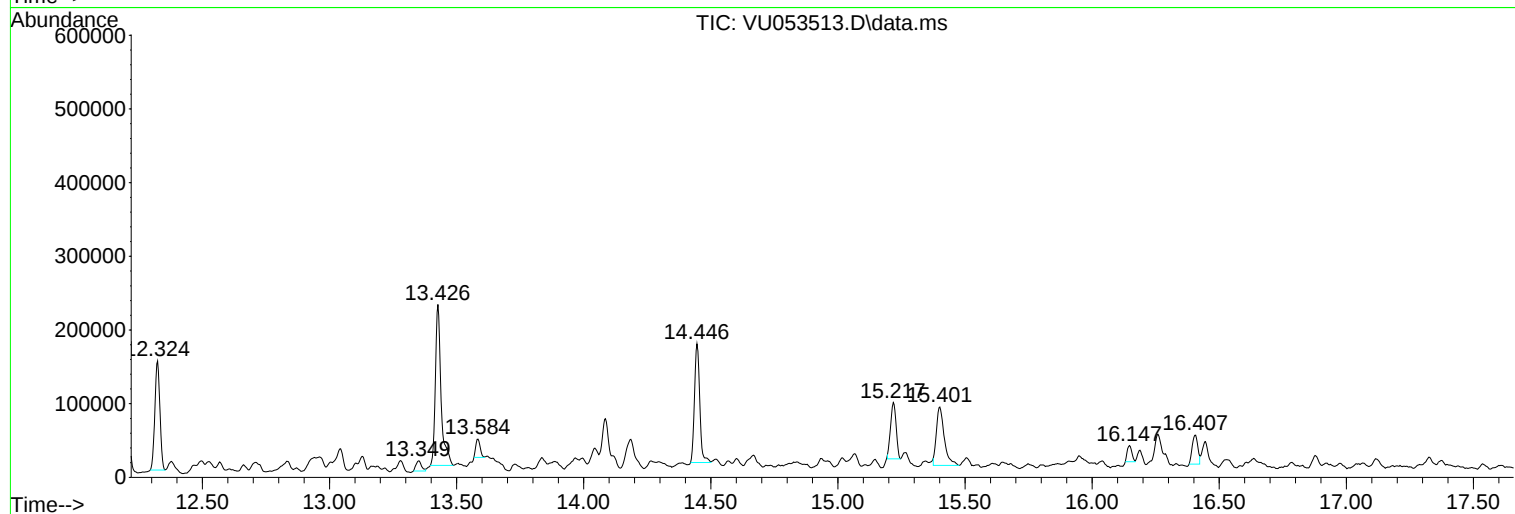
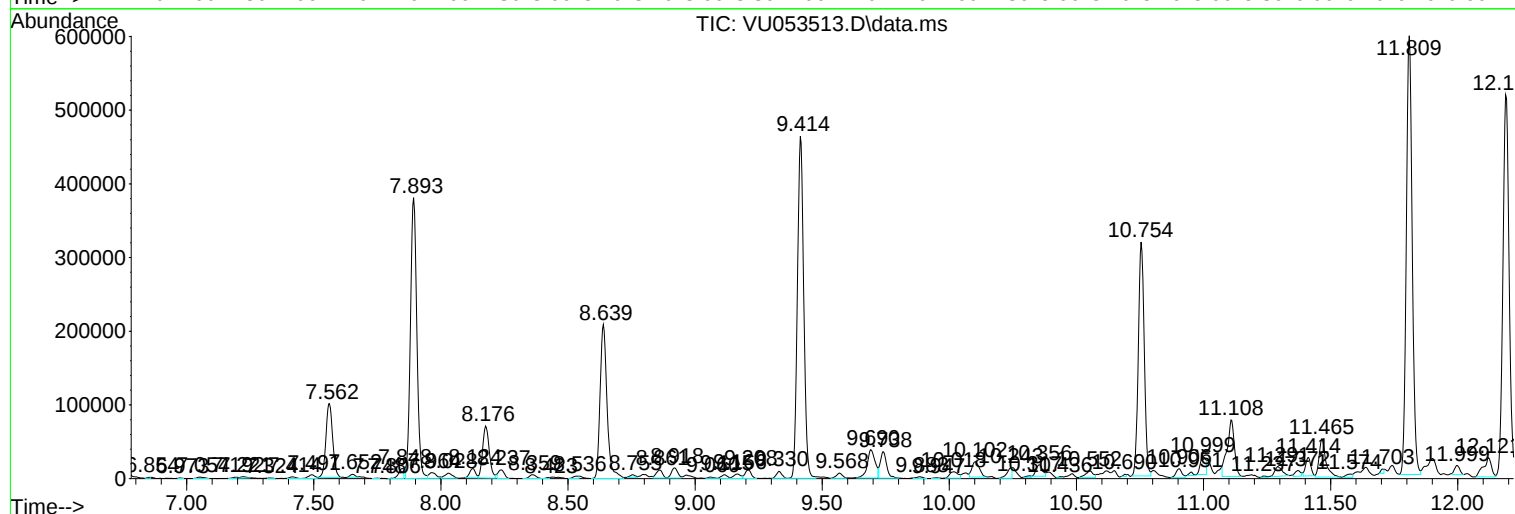
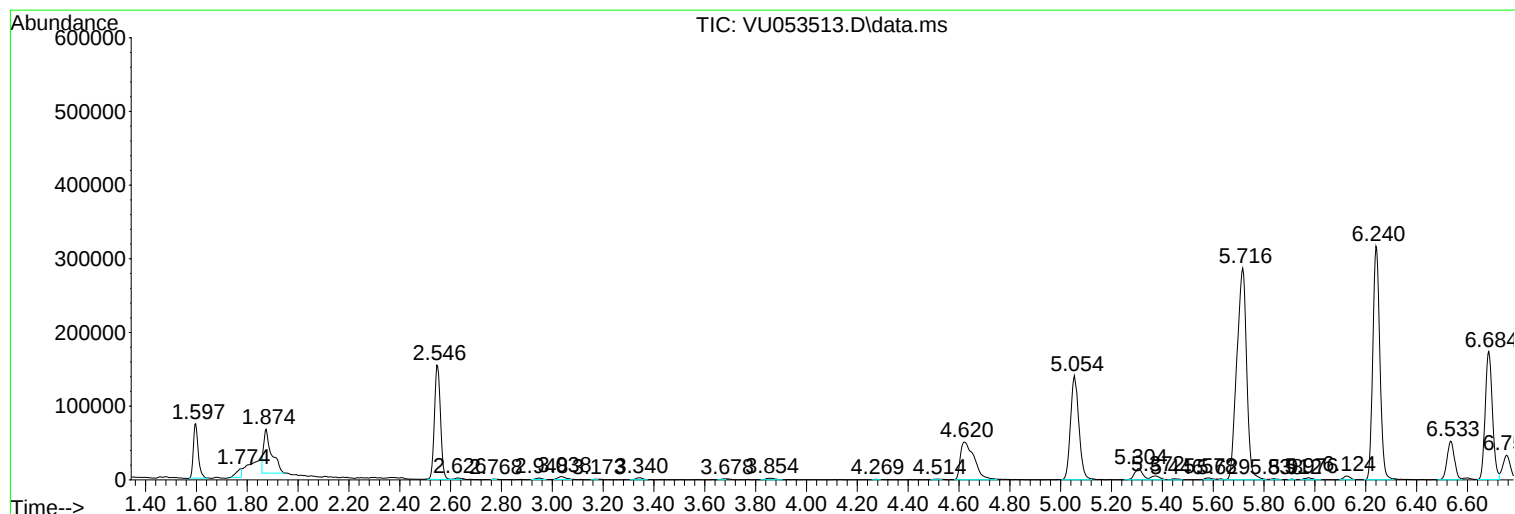
Sum of corrected areas: 9713044

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ALS Vial : 6 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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ALS Vial : 6 Sample Multiplier: 1

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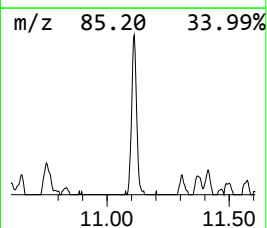
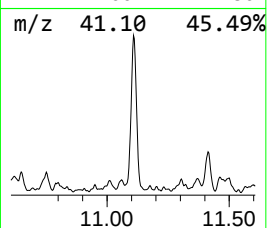
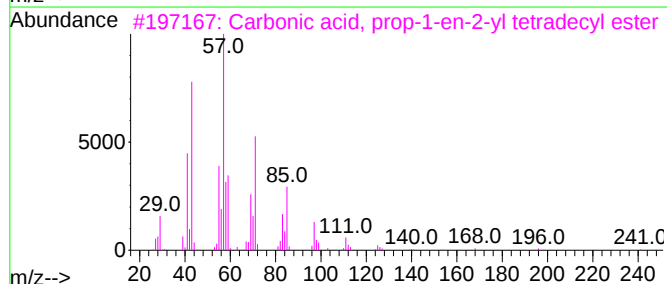
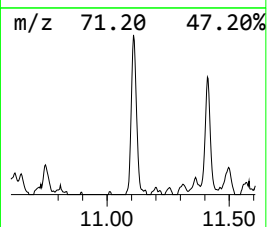
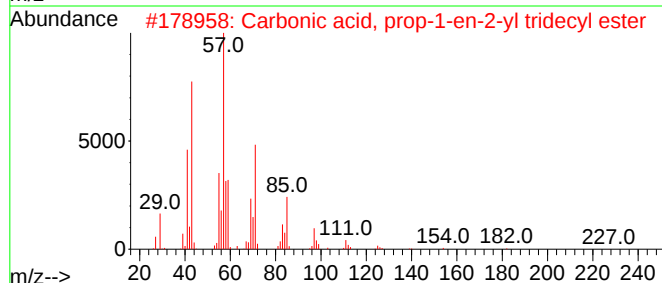
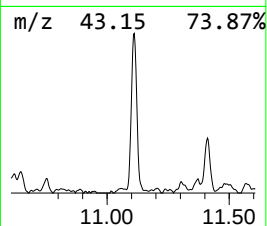
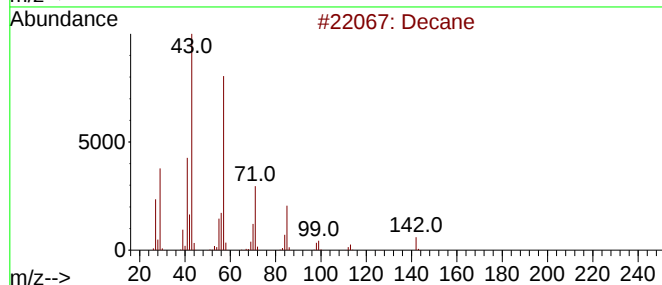
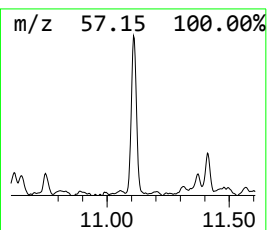
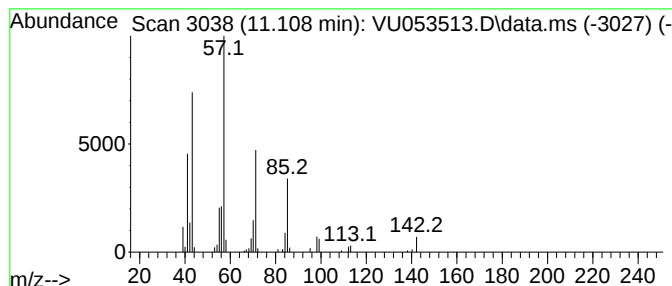
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.108	7.94 ug/L	150507	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane	142	C10H22	000124-18-5	94
2			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	90
3			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	83
4			Decane	142	C10H22	000124-18-5	81
5			Pentadecane	212	C15H32	000629-62-9	72



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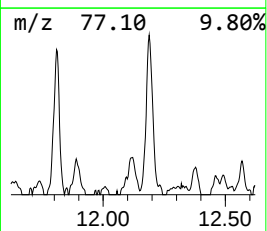
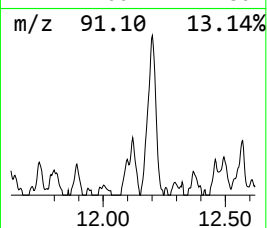
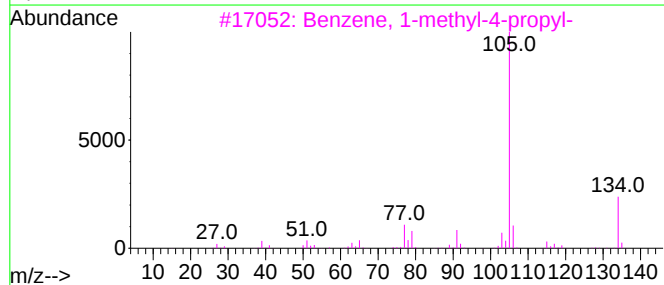
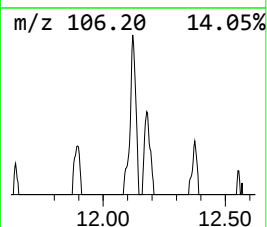
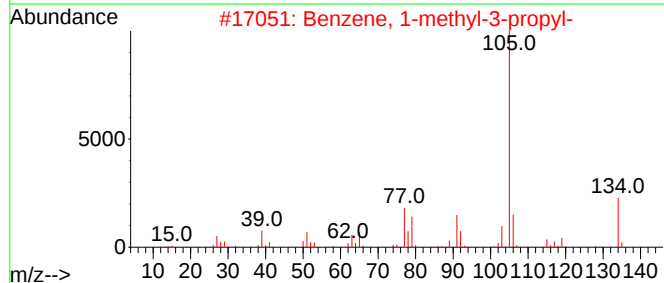
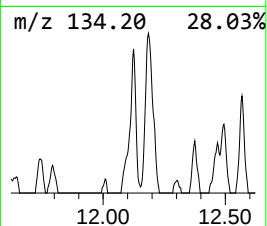
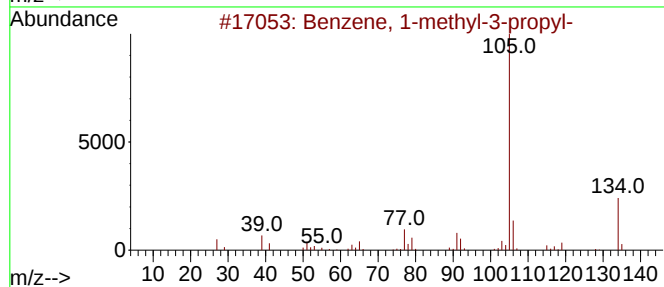
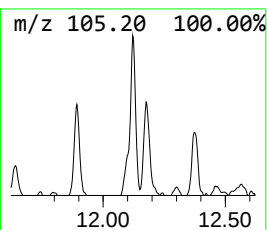
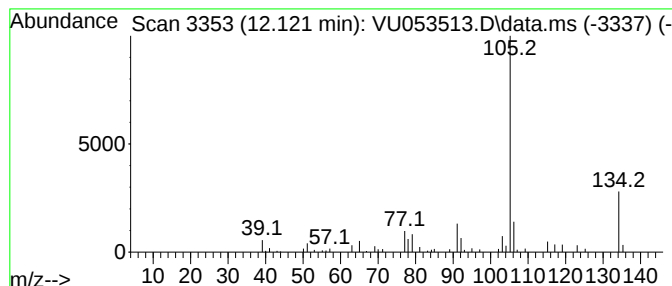
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Benzene, 1-methyl-3-propyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.121	3.03 ug/L	57374	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-3-propyl-	134	C10H14	001074-43-7	94
2			Benzene, 1-methyl-3-propyl-	134	C10H14	001074-43-7	91
3			Benzene, 1-methyl-4-propyl-	134	C10H14	001074-55-1	91
4			Benzene, 1-methyl-3-propyl-	134	C10H14	001074-43-7	91
5			Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	91



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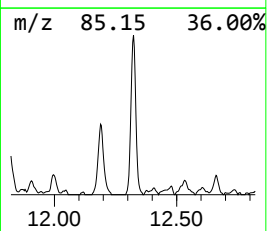
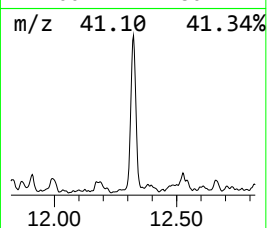
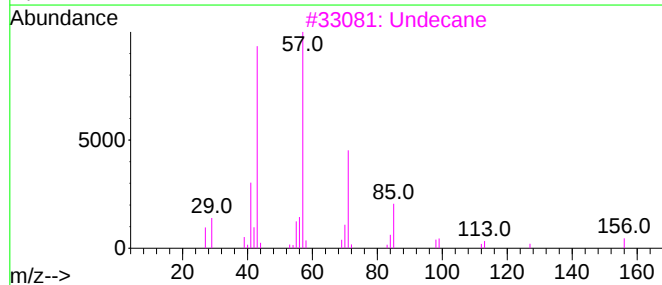
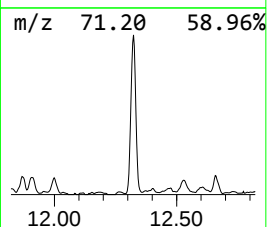
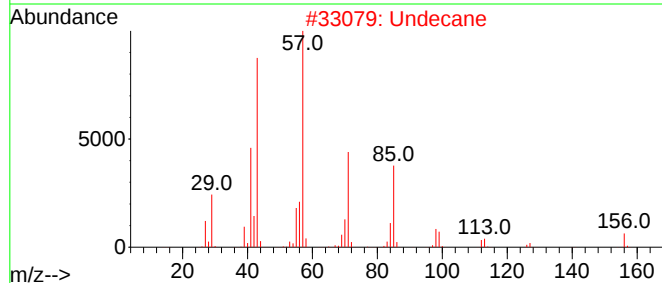
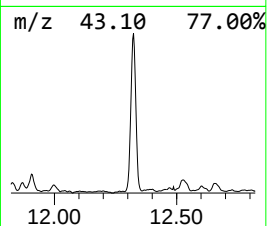
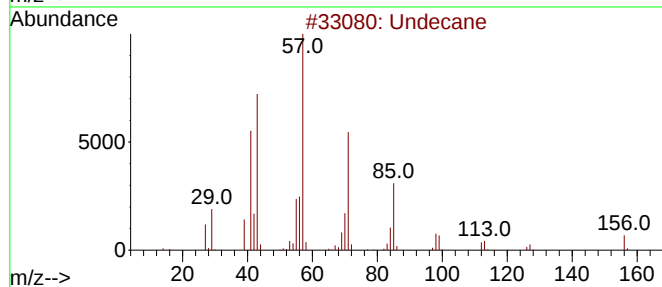
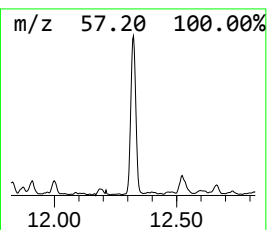
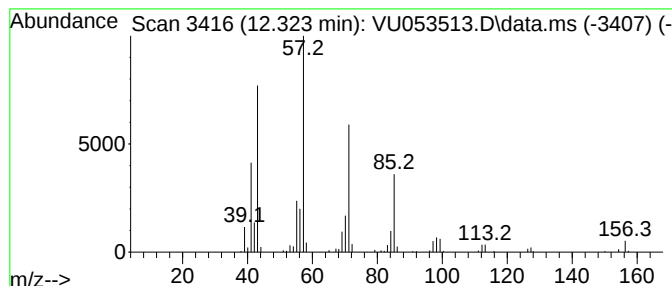
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.323	10.70 ug/L	202752	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	Hexadecane			226	C16H34	000544-76-3	90
5	Tetradecane			198	C14H30	000629-59-4	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040323\
Data File : VU053513.D
Acq On : 03 Apr 2023 12:30
Operator : JC/MD
Sample : 02121-15ME
Misc : 3.42g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C1188ME

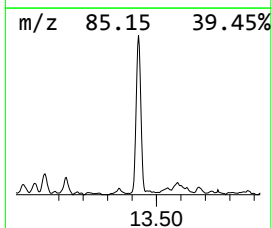
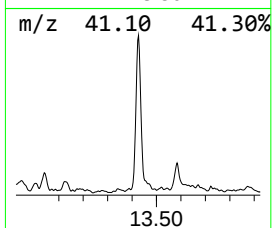
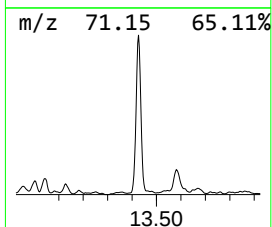
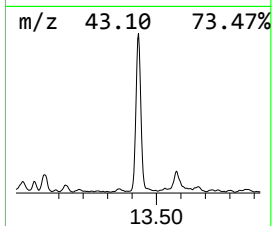
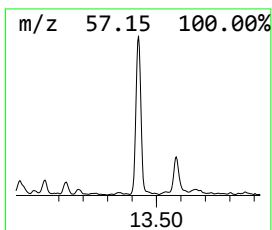
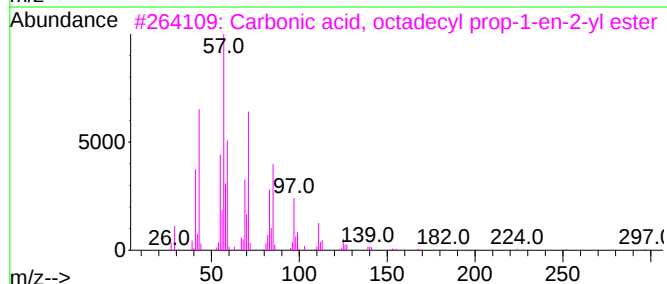
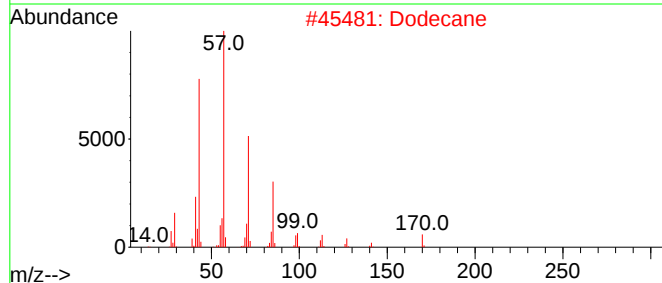
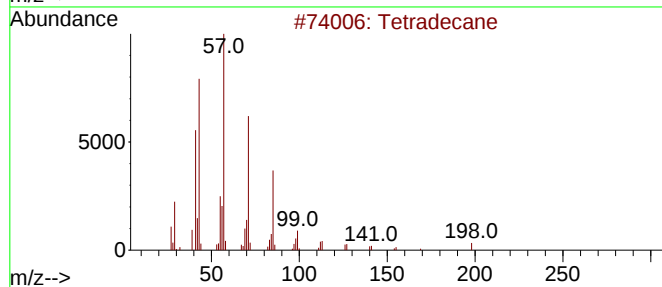
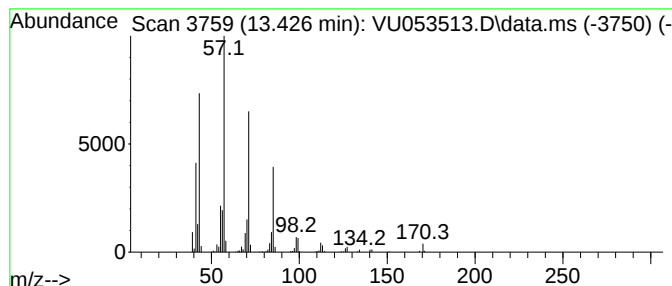
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Quant Title : VOC Analysis

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.426	18.07 ug/L	342476	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	91
2			Dodecane	170	C12H26	000112-40-3	90
3			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	90
4			Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	86
5			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040323\
Data File : VU053513.D
Acq On : 03 Apr 2023 12:30
Operator : JC/MD
Sample : 02121-15ME
Misc : 3.42g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C1188ME

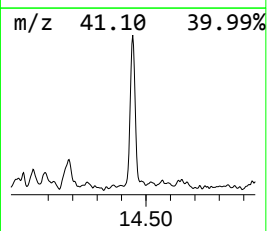
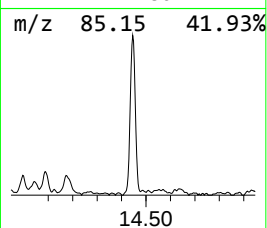
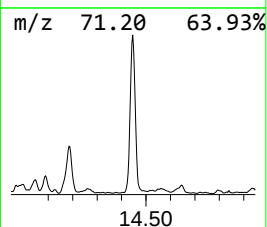
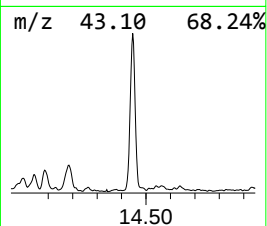
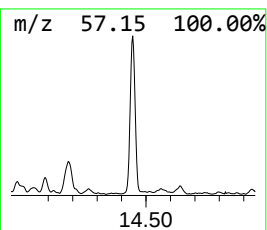
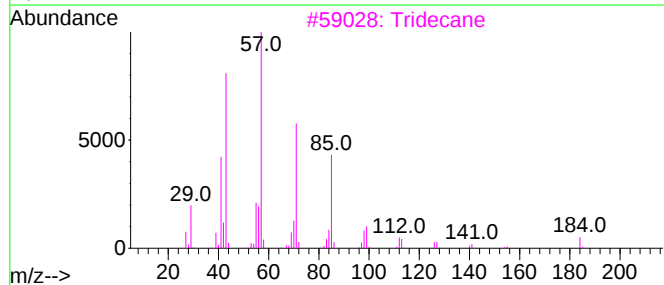
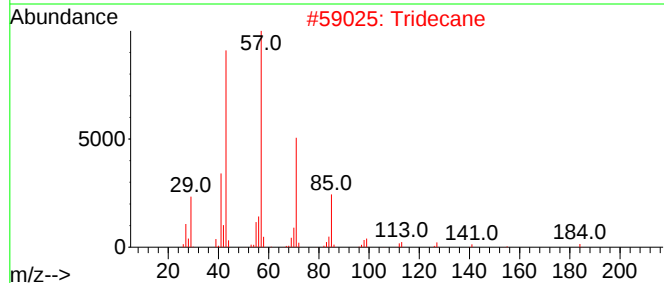
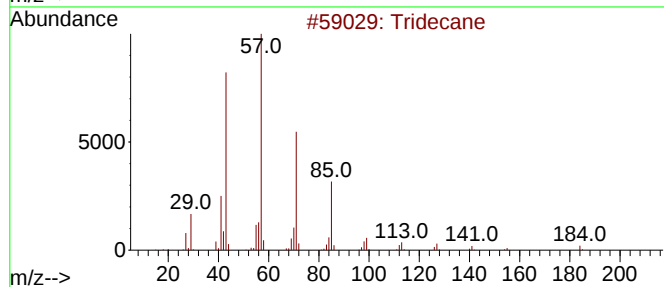
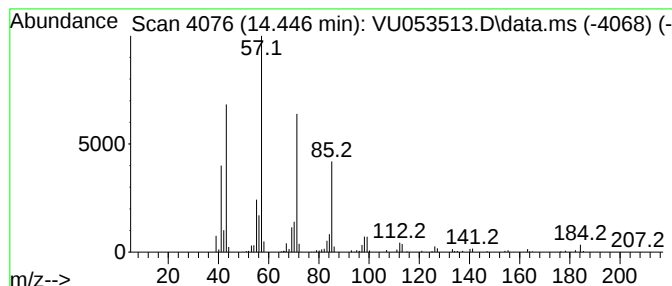
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Quant Title : VOC Analysis

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.446	12.18 ug/L	230792	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	94
2			Tridecane	184	C13H28	000629-50-5	91
3			Tridecane	184	C13H28	000629-50-5	90
4			Dodecane	170	C12H26	000112-40-3	86
5			Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040323\
Data File : VU053513.D
Acq On : 03 Apr 2023 12:30
Operator : JC/MD
Sample : 02121-15ME
Misc : 3.42g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C1188ME

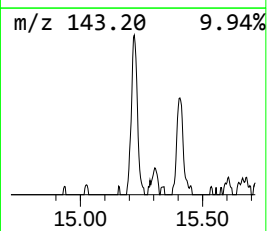
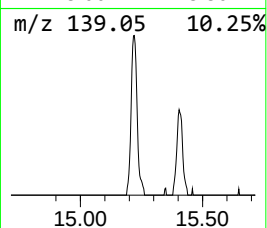
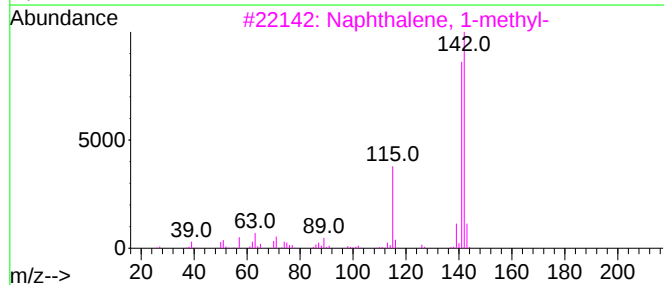
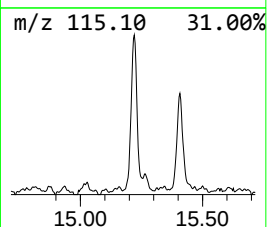
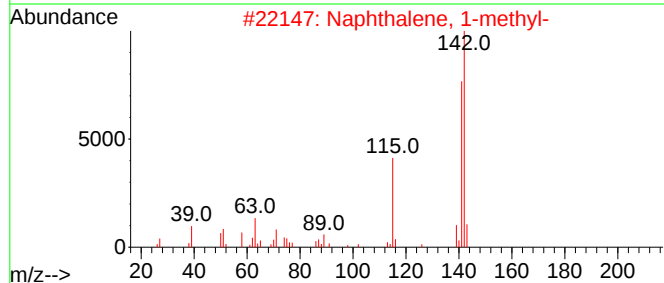
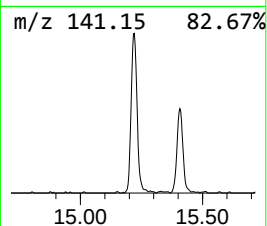
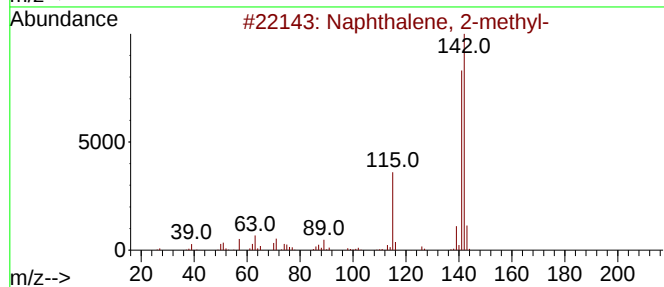
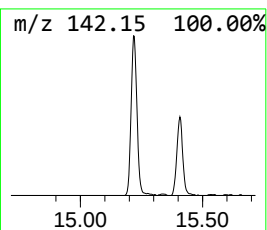
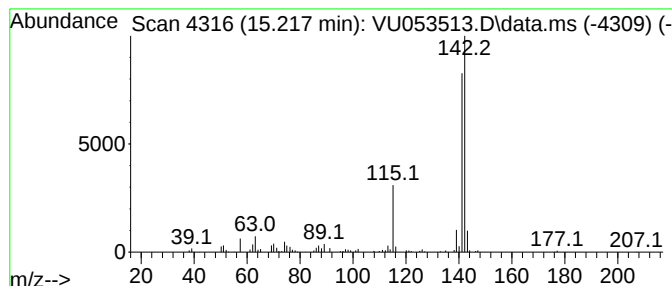
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Quant Title : VOC Analysis

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

Peak Number 7 Naphthalene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.217	6.10 ug/L	115620	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
3			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
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\VU040323\
Data File : VU053513.D
Acq On : 03 Apr 2023 12:30
Operator : JC/MD
Sample : 02121-15ME
Misc : 3.42g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C1188ME

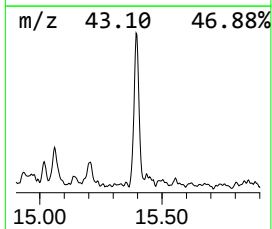
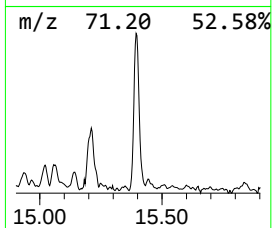
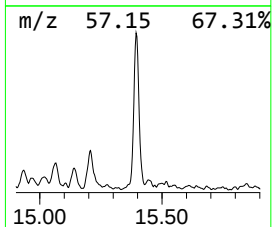
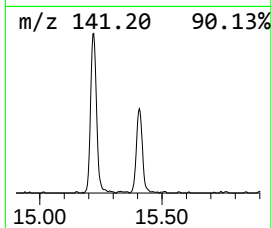
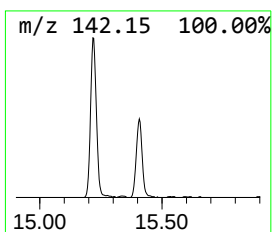
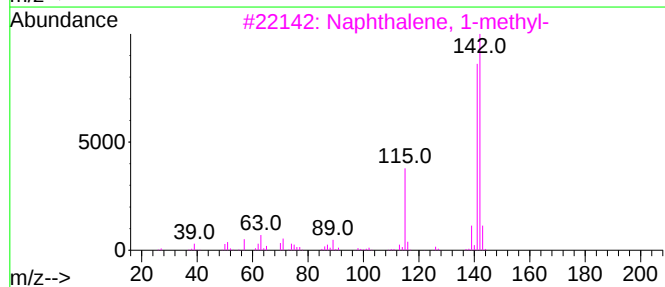
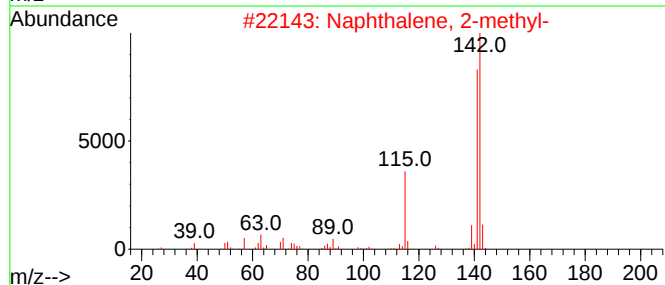
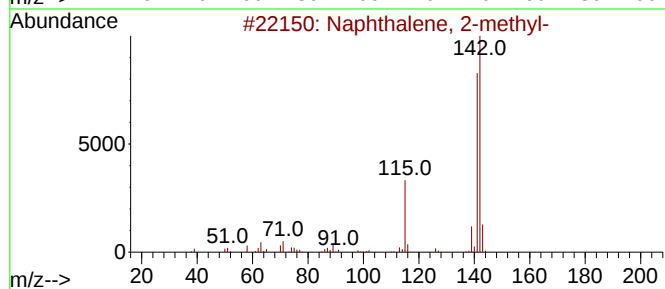
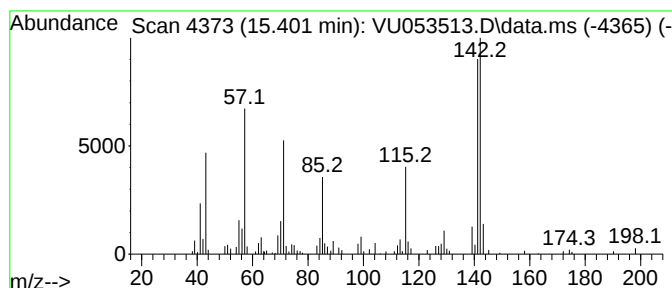
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Quant Title : VOC Analysis

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

Peak Number 8 Naphthalene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.401	8.98 ug/L	170138	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	93
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	93
3			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	93
4			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	89
5			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040323\
Data File : VU053513.D
Acq On : 03 Apr 2023 12:30
Operator : JC/MD
Sample : 02121-15ME
Misc : 3.42g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C1188ME

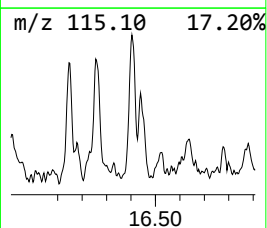
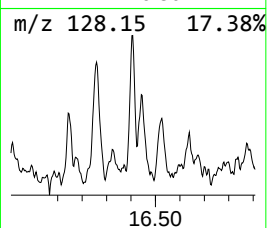
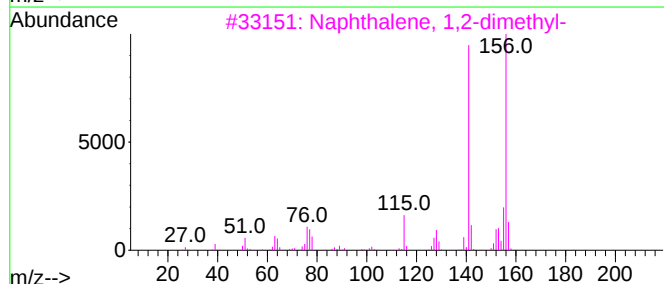
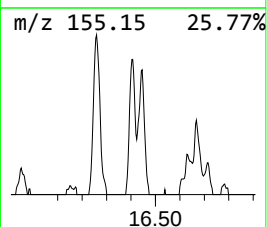
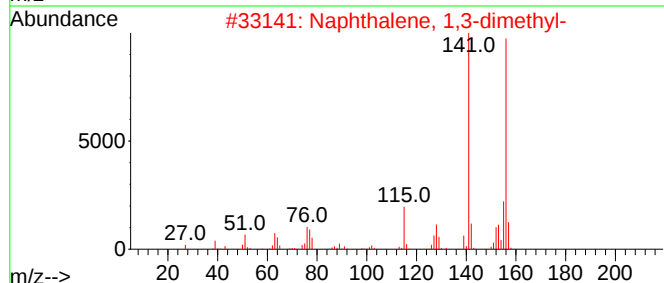
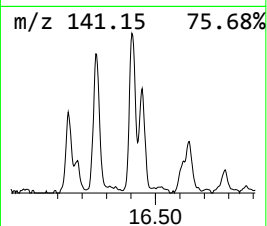
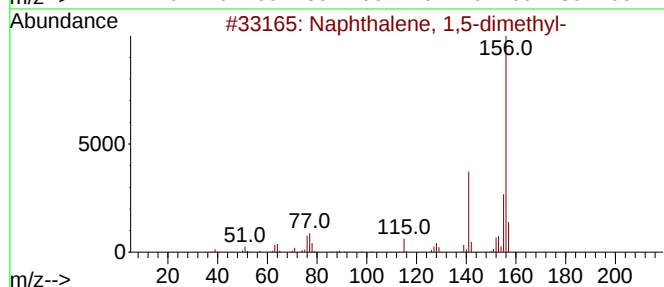
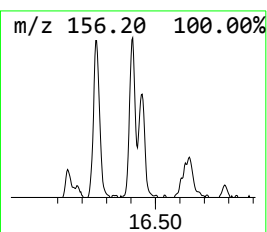
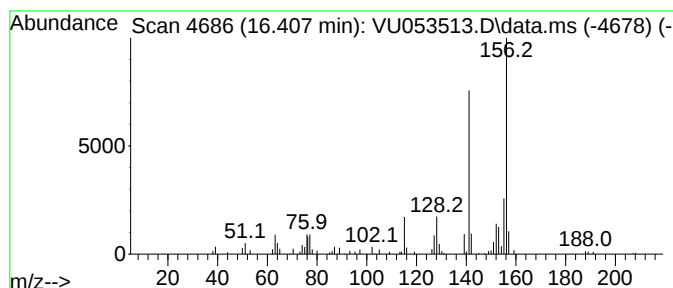
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Quant Title : VOC Analysis

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

Peak Number 9 Naphthalene, 1,5-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.407	3.19 ug/L	60415	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	96
2			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96
3			Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	96
4			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	95
5			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040323\
Data File : VU053513.D
Acq On : 03 Apr 2023 12:30
Operator : JC/MD
Sample : 02121-15ME
Misc : 3.42g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 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\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	11.108	7.9	ug/L	150507	3	11.809	947750	50.0
Benzene, 1-meth...	12.121	3.0	ug/L	57374	3	11.809	947750	50.0
(DEL) Alkane: S...	12.323	10.7	ug/L	202752	3	11.809	947750	50.0
(DEL) Alkane: S...	13.426	18.1	ug/L	342476	3	11.809	947750	50.0
(DEL) Alkane: S...	14.446	12.2	ug/L	230792	3	11.809	947750	50.0
Naphthalene, 2-...	15.217	6.1	ug/L	115620	3	11.809	947750	50.0
Naphthalene, 1-...	15.401	9.0	ug/L	170138	3	11.809	947750	50.0
Naphthalene, 1,...	16.407	3.2	ug/L	60415	3	11.809	947750	50.0