

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033123\
 Data File : VU053499.D
 Acq On : 31 Mar 2023 18:11
 Operator : JC/MD
 Sample : 02121-15ME
 Misc : 3.42g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 16 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: VU053499.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	33	37	42	rBV3	3469	3925	0.20%	0.023%
2	1.597	71	80	102	rBV	212707	310493	15.89%	1.819%
3	1.774	122	135	136	rBV6	10449	15449	0.79%	0.091%
4	1.871	160	165	181	rVB	70209	92209	4.72%	0.540%
5	2.540	361	373	393	rBV	453054	735493	37.64%	4.310%
6	2.626	397	400	402	rBV2	1233	875	0.04%	0.005%
7	2.765	439	443	449	rBV	1080	968	0.05%	0.006%
8	2.945	492	499	503	rBV4	2005	2631	0.13%	0.015%
9	3.031	512	526	545	rVB9	5058	14477	0.74%	0.085%
10	3.112	546	551	552	rBV2	572	459	0.02%	0.003%
11	3.170	563	569	571	rBV2	1464	1347	0.07%	0.008%
12	3.340	611	622	632	rVB7	4374	8678	0.44%	0.051%
13	3.559	684	690	695	rBV2	438	534	0.03%	0.003%
14	3.671	717	725	726	rBV5	2831	2881	0.15%	0.017%
15	3.858	770	783	790	rBV6	2849	5616	0.29%	0.033%
16	4.279	904	914	918	rBV5	1000	1663	0.09%	0.010%
17	4.517	979	988	997	rVB7	1322	2599	0.13%	0.015%
18	4.620	1008	1020	1064	rBV	120972	413695	21.17%	2.424%
19	5.054	1138	1155	1182	rBV	347994	805743	41.23%	4.722%
20	5.305	1219	1233	1243	rBV2	14742	33299	1.70%	0.195%
21	5.436	1269	1274	1275	rBV2	1039	804	0.04%	0.005%
22	5.581	1310	1319	1327	rBV6	3945	8139	0.42%	0.048%
23	5.713	1339	1360	1393	rBV2	739362	1944505	99.51%	11.395%
24	5.970	1432	1440	1441	rBV2	2679	3007	0.15%	0.018%
25	6.128	1475	1489	1501	rBV6	7668	14596	0.75%	0.086%
26	6.240	1510	1524	1548	rBV	383157	749802	38.37%	4.394%
27	6.334	1552	1553	1562	rVB4	935	894	0.05%	0.005%
28	6.391	1569	1571	1581	rVB3	461	529	0.03%	0.003%
29	6.533	1600	1615	1629	rBV3	67284	139622	7.15%	0.818%
30	6.684	1646	1662	1676	rBV	434782	858210	43.92%	5.029%
31	6.854	1709	1715	1721	rVB5	2099	2653	0.14%	0.016%
32	6.973	1744	1752	1759	rBV6	1079	1611	0.08%	0.009%
33	7.054	1765	1777	1790	rVB7	2194	5321	0.27%	0.031%
34	7.192	1812	1820	1824	rBV6	1733	2889	0.15%	0.017%
35	7.231	1827	1832	1838	rVB4	2428	2710	0.14%	0.016%
36	7.334	1856	1864	1870	rBV5	1044	1566	0.08%	0.009%

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Integrator: RTE

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Stop Thrs : 0

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

37	7.420	1883	1891	1899	rVB5	2097	3131	0.16%	0.018%
38	7.491	1903	1913	1920	rBV4	5076	8717	0.45%	0.051%
39	7.559	1920	1934	1953	rVV	252222	468678	23.98%	2.746%
40	7.655	1956	1964	1971	rBV3	4274	6774	0.35%	0.040%
41	7.732	1985	1988	1993	rBV3	461	459	0.02%	0.003%
42	7.848	2006	2024	2026	rBV3	15829	23511	1.20%	0.138%
43	7.893	2026	2038	2054	rVB	965958	1703838	87.19%	9.984%
44	8.089	2096	2099	2100	rBV2	1016	547	0.03%	0.003%
45	8.124	2100	2110	2116	rVV3	16090	23743	1.22%	0.139%
46	8.176	2116	2126	2140	rVV	162761	303425	15.53%	1.778%
47	8.359	2173	2183	2193	rVB6	5930	10421	0.53%	0.061%
48	8.411	2193	2199	2200	rBV2	539	622	0.03%	0.004%
49	8.430	2200	2205	2207	rBV5	1601	1334	0.07%	0.008%
50	8.539	2229	2239	2252	rVB10	4588	9233	0.47%	0.054%
51	8.642	2256	2271	2298	rBV	493506	947584	48.49%	5.553%
52	8.755	2299	2306	2312	rBV6	3345	4884	0.25%	0.029%
53	8.861	2332	2339	2347	rVB3	10877	16906	0.87%	0.099%
54	8.919	2348	2357	2366	rBV3	13297	22251	1.14%	0.130%
55	9.060	2391	2401	2406	rBV6	1972	2948	0.15%	0.017%
56	9.118	2410	2419	2424	rBV4	4793	7161	0.37%	0.042%
57	9.166	2426	2434	2439	rVV6	5212	9065	0.46%	0.053%
58	9.205	2440	2446	2458	rVB4	12179	20749	1.06%	0.122%
59	9.330	2474	2485	2497	rBV4	9642	15878	0.81%	0.093%
60	9.417	2497	2512	2530	rBV	522844	944510	48.33%	5.535%
61	9.568	2551	2559	2569	rVV3	6084	10612	0.54%	0.062%
62	9.694	2579	2598	2606	rBV3	34466	79313	4.06%	0.465%
63	9.739	2607	2612	2637	rVB	40000	68348	3.50%	0.401%
64	9.854	2644	2648	2649	rBV	649	485	0.02%	0.003%
65	9.883	2652	2657	2666	rVB6	2329	3123	0.16%	0.018%
66	9.941	2666	2675	2678	rBV3	860	895	0.05%	0.005%
67	10.015	2685	2698	2702	rBV6	9155	16682	0.85%	0.098%
68	10.105	2718	2726	2739	rVB3	19637	38204	1.96%	0.224%
69	10.195	2751	2754	2756	rBV2	627	421	0.02%	0.002%
70	10.243	2756	2769	2785	rVV9	13574	32079	1.64%	0.188%
71	10.353	2794	2803	2811	rBV6	14940	27601	1.41%	0.162%
72	10.481	2838	2843	2852	rVB3	4996	7313	0.37%	0.043%
73	10.555	2852	2866	2875	rBV9	8732	22347	1.14%	0.131%
74	10.690	2902	2908	2914	rBV6	3755	5455	0.28%	0.032%
75	10.755	2916	2928	2940	rBV	732032	1174722	60.12%	6.884%
76	10.903	2962	2974	2981	rBV2	12792	21079	1.08%	0.124%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

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Filtering: 5

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 Title : VOC Analysis

77	10.951	2983	2989	2994	rBV7	5054	6737	0.34%	0.039%
78	10.999	2996	3004	3008	rBV2	20874	32035	1.64%	0.188%
79	11.108	3027	3038	3052	rVB2	82927	157523	8.06%	0.923%
80	11.240	3073	3079	3081	rBV4	2267	2352	0.12%	0.014%
81	11.295	3088	3096	3110	rBV6	11860	24394	1.25%	0.143%
82	11.411	3126	3132	3140	rVB2	24010	32457	1.66%	0.190%
83	11.465	3140	3149	3174	rVB	48412	93711	4.80%	0.549%
84	11.568	3175	3181	3184	rBV5	4638	5107	0.26%	0.030%
85	11.809	3244	3256	3270	rBV	712283	1122517	57.44%	6.578%
86	12.095	3336	3345	3347	rBV7	11760	15094	0.77%	0.088%
87	12.189	3362	3374	3394	rBV	1198315	1954116	100.00%	11.451%
88	12.324	3407	3416	3426	rBV	149158	207594	10.62%	1.216%
89	12.465	3454	3460	3463	rBV3	8275	10683	0.55%	0.063%
90	12.665	3517	3522	3527	rBV5	6620	7829	0.40%	0.046%
91	13.349	3728	3735	3743	rBV3	12977	22613	1.16%	0.133%
92	13.427	3751	3759	3779	rVB	205641	329683	16.87%	1.932%
93	13.584	3802	3808	3815	rBV3	24839	35618	1.82%	0.209%
94	13.832	3880	3885	3893	rBV6	12939	21830	1.12%	0.128%
95	14.086	3959	3964	3972	rVB	48556	62559	3.20%	0.367%
96	14.182	3984	3994	4011	rVB7	35160	82821	4.24%	0.485%
97	14.446	4068	4076	4091	rBV	157038	220403	11.28%	1.292%
98	15.217	4306	4316	4325	rBV	77675	140404	7.19%	0.823%
99	15.398	4365	4372	4389	rVB3	90572	167049	8.55%	0.979%
100	16.404	4679	4685	4692	rBV3	40083	55222	2.83%	0.324%

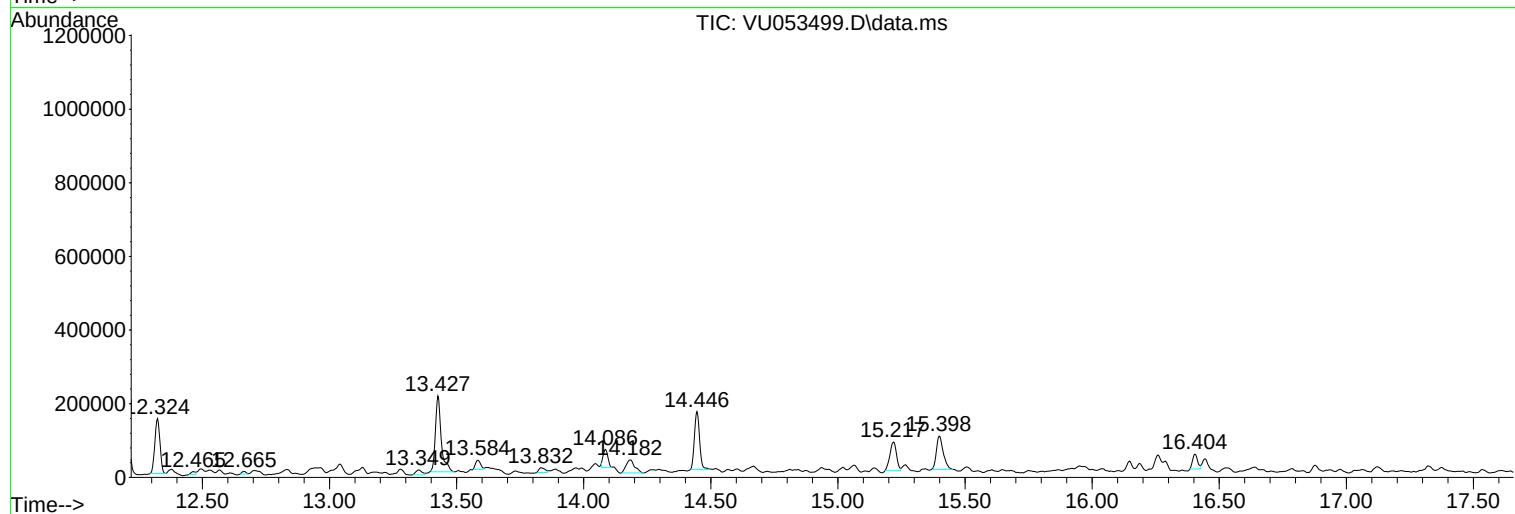
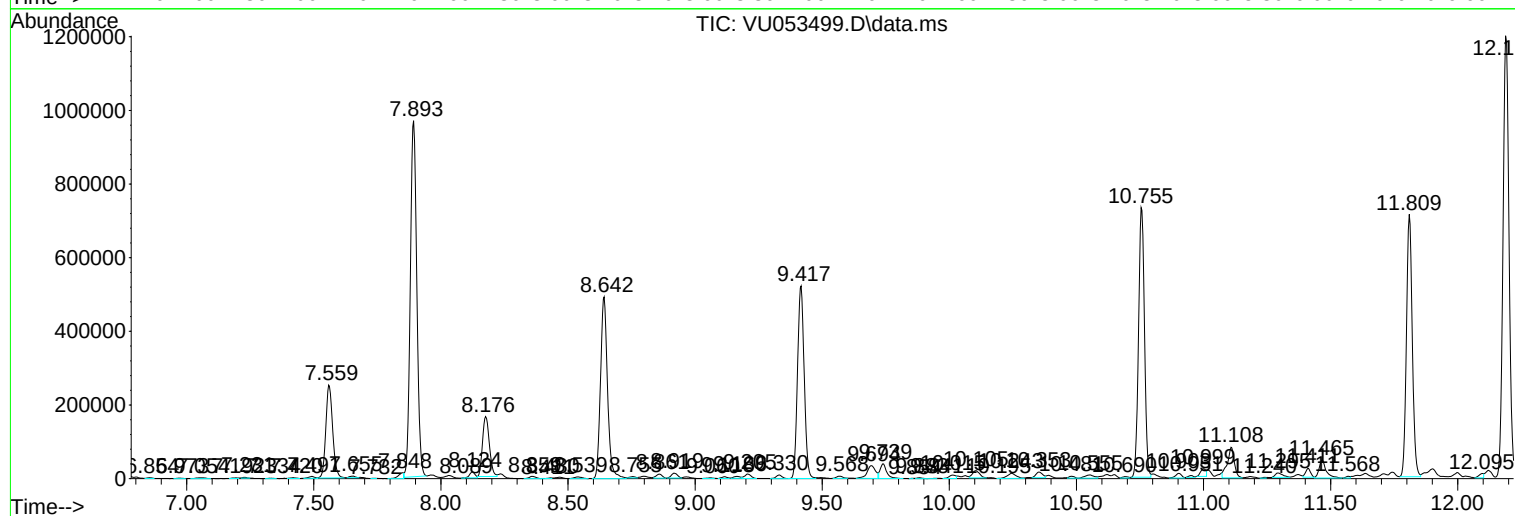
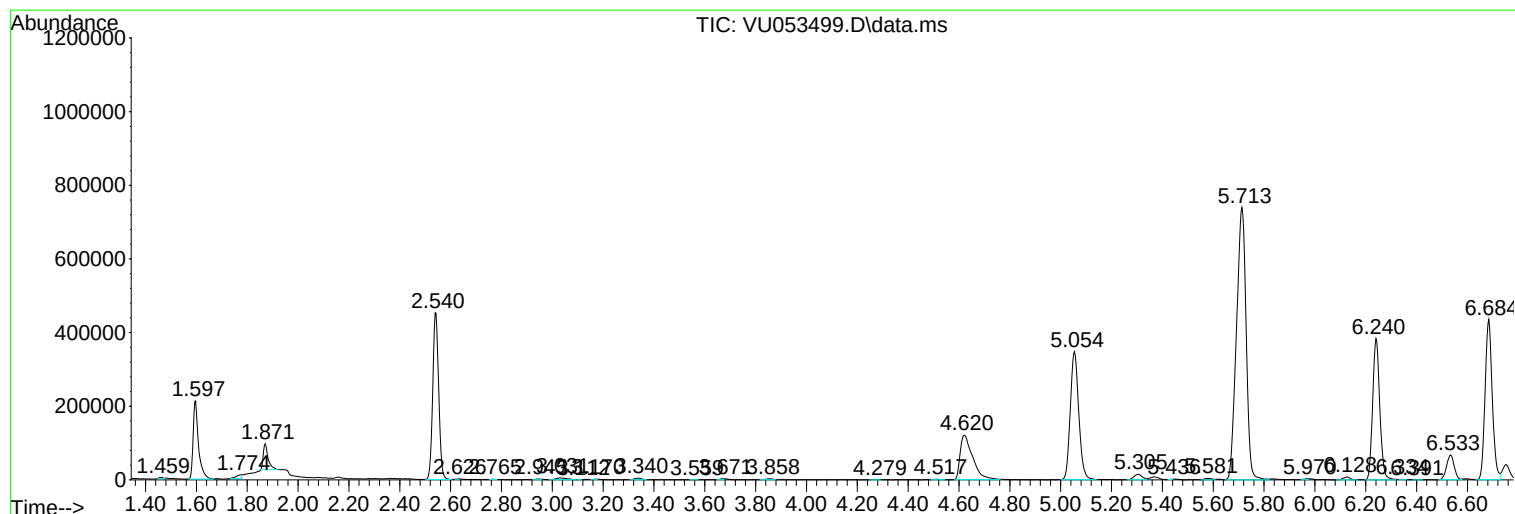
Sum of corrected areas: 17065291

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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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C1188ME

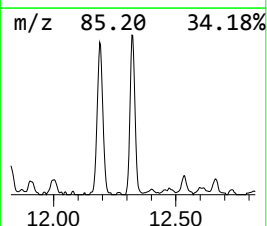
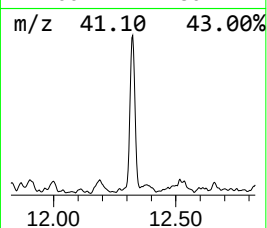
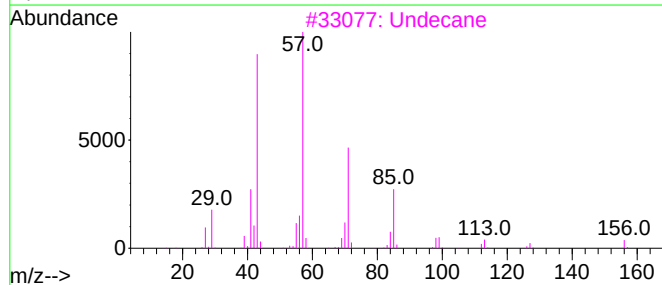
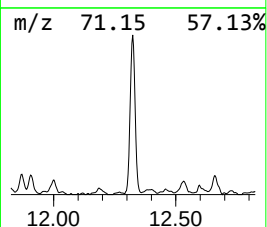
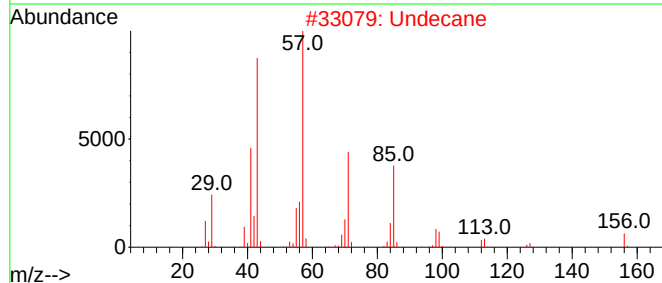
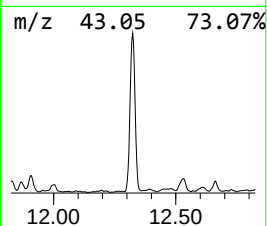
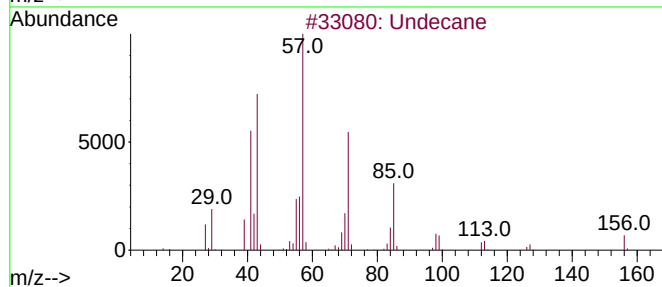
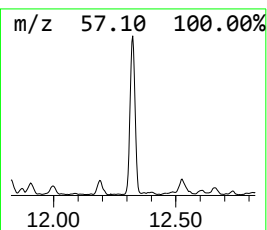
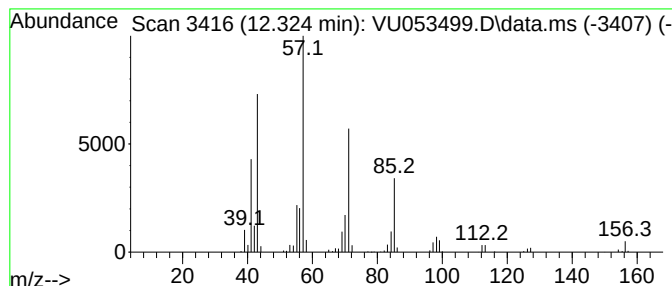
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.324	9.25 ug/L	207594	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	91



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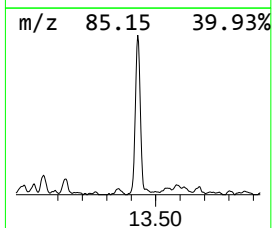
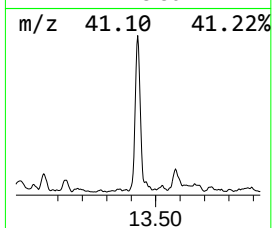
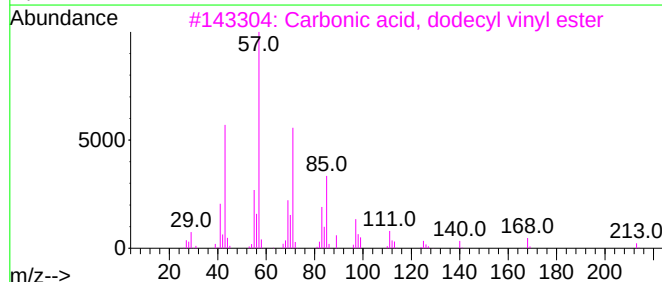
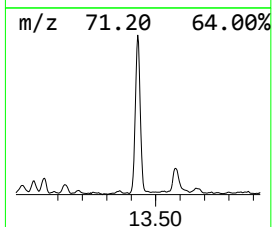
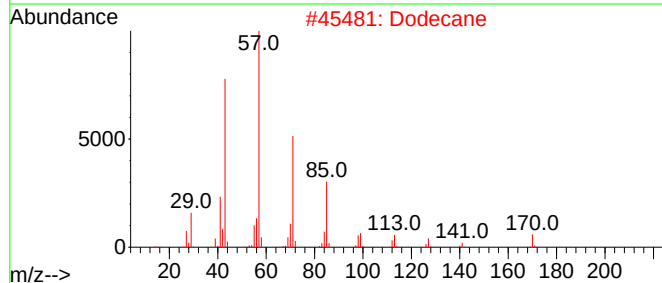
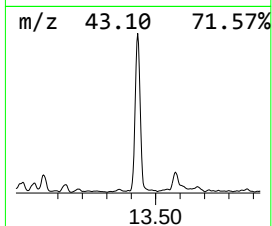
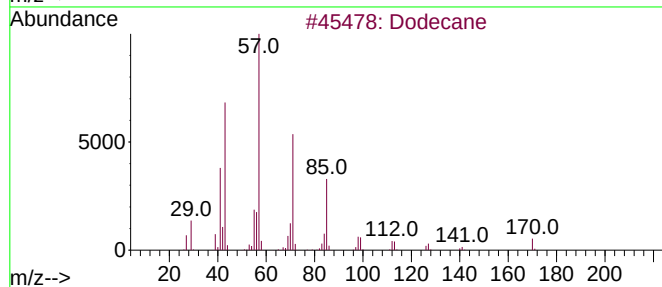
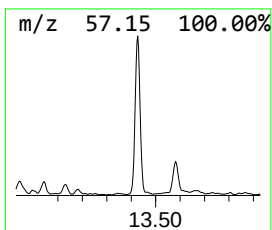
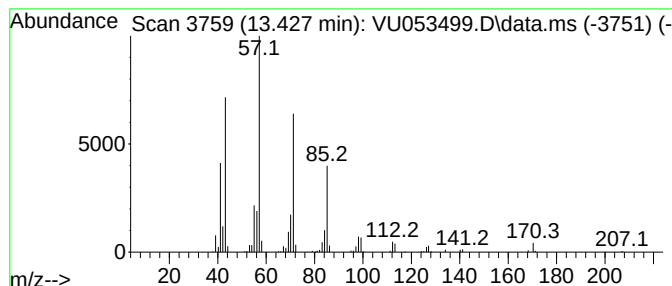
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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.
13.427	14.69 ug/L	329683	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	90
3			Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	90
4			Tetradecane	198	C14H30	000629-59-4	90
5			Tetradecane	198	C14H30	000629-59-4	86



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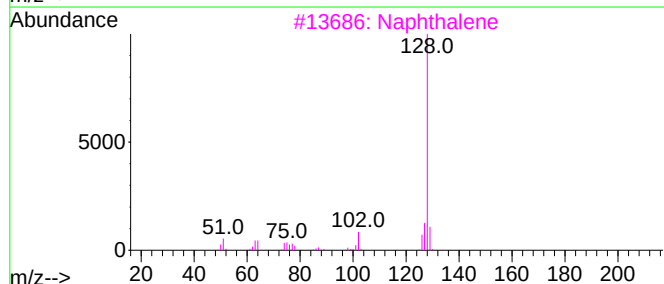
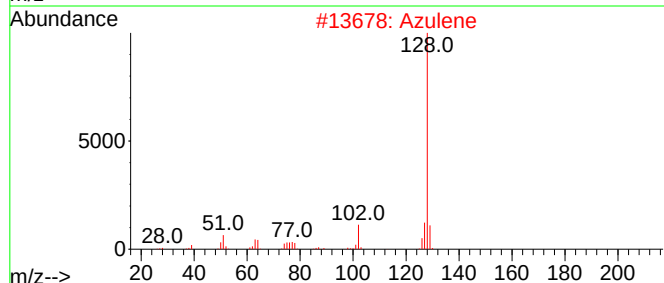
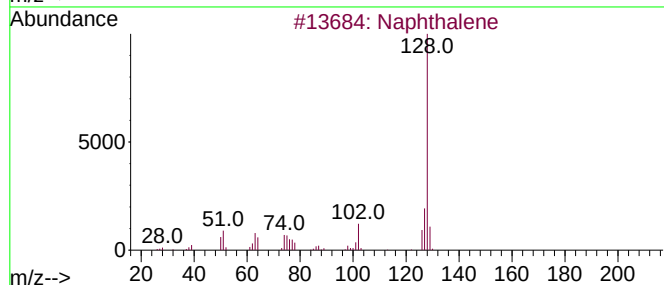
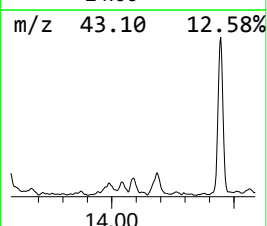
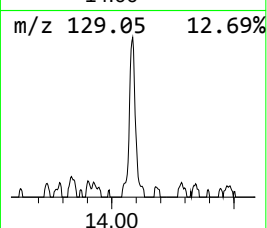
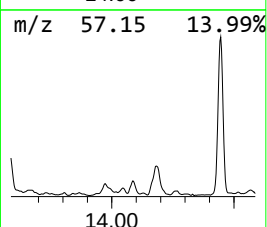
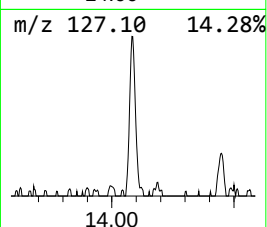
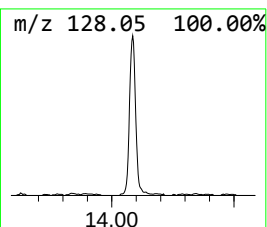
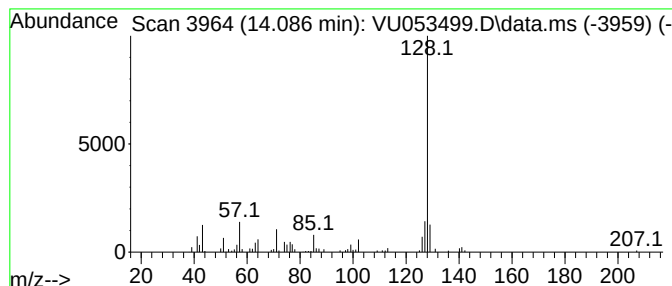
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Quant Title : VOC Analysis

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

Peak Number 4 Azulene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.086	2.79 ug/L	62559	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	83
2			Azulene	128	C10H8	000275-51-4	81
3			Naphthalene	128	C10H8	000091-20-3	81
4			Naphthalene	128	C10H8	000091-20-3	74
5			Naphthalene	128	C10H8	000091-20-3	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033123\
Data File : VU053499.D
Acq On : 31 Mar 2023 18:11
Operator : JC/MD
Sample : 02121-15ME
Misc : 3.42g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C1188ME

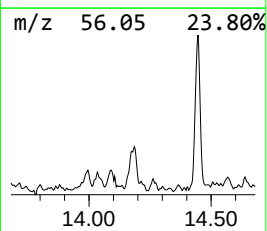
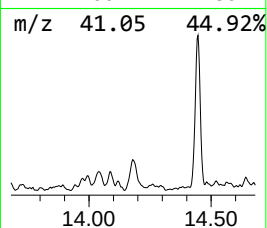
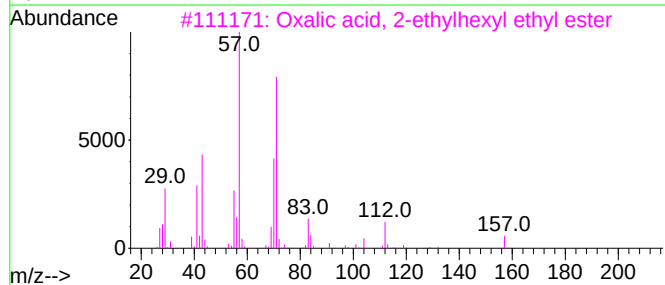
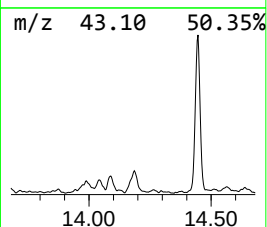
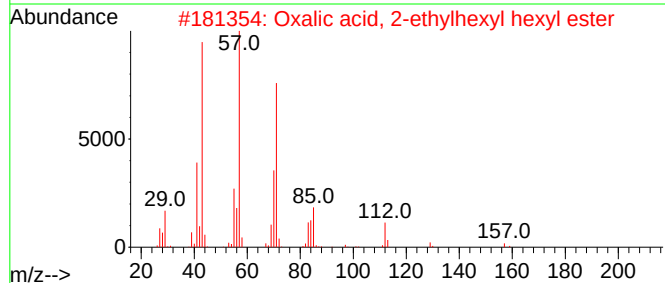
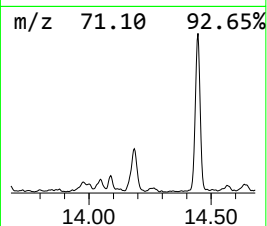
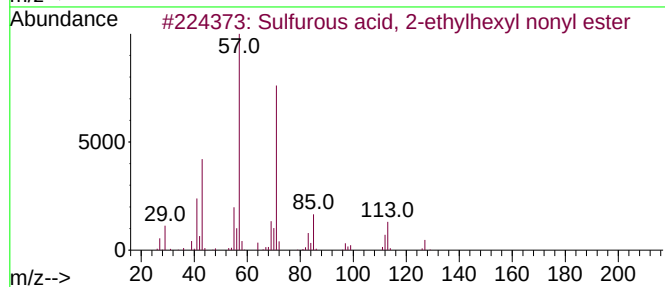
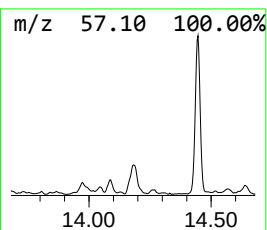
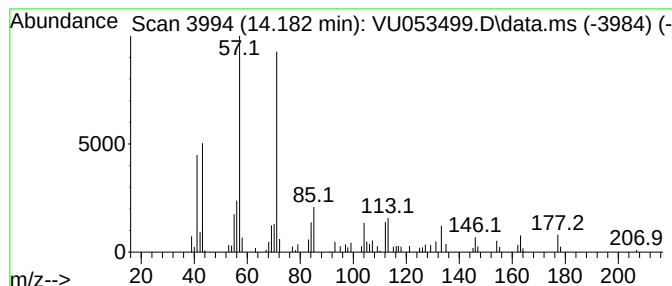
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Quant Title : VOC Analysis

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

Peak Number 5 Sulfurous acid, 2-ethylhexy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.182	3.69 ug/L	82821	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1010309-19-2	64
2			Oxalic acid, 2-ethylhexyl hexyl ...	286	C16H30O4	1000309-38-9	64
3			Oxalic acid, 2-ethylhexyl ethyl ...	230	C12H22O4	1000309-38-4	53
4			Decane, 3,4-dimethyl-	170	C12H26	017312-45-7	50
5			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033123\
Data File : VU053499.D
Acq On : 31 Mar 2023 18:11
Operator : JC/MD
Sample : 02121-15ME
Misc : 3.42g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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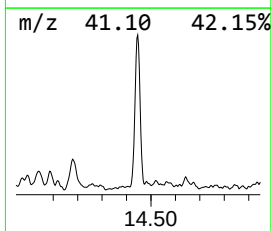
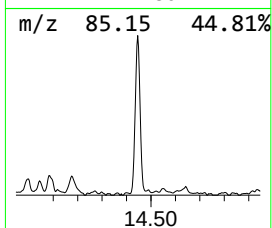
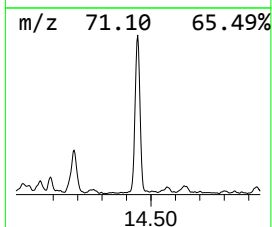
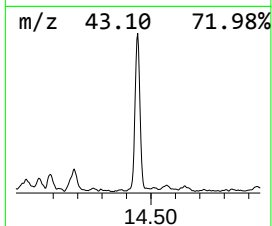
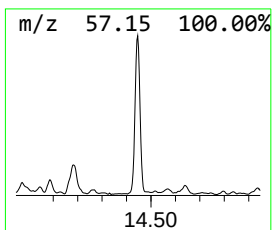
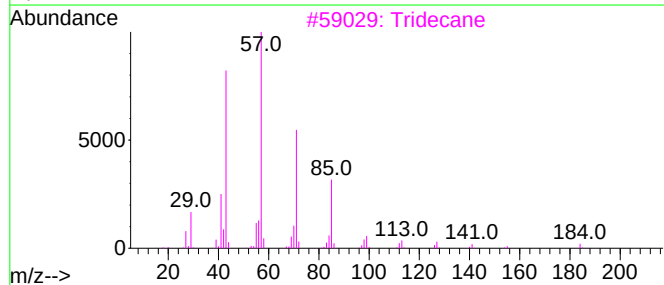
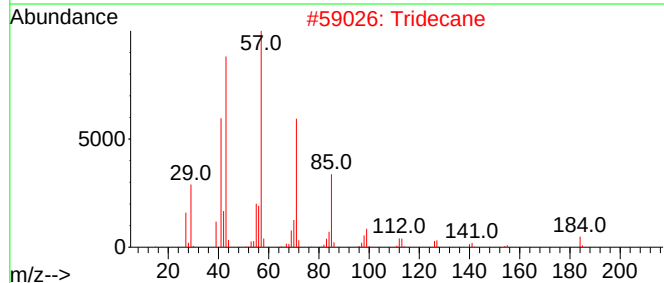
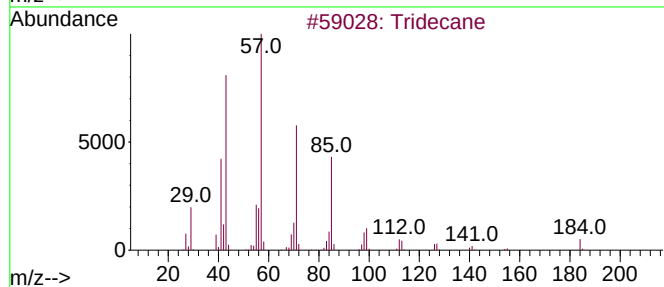
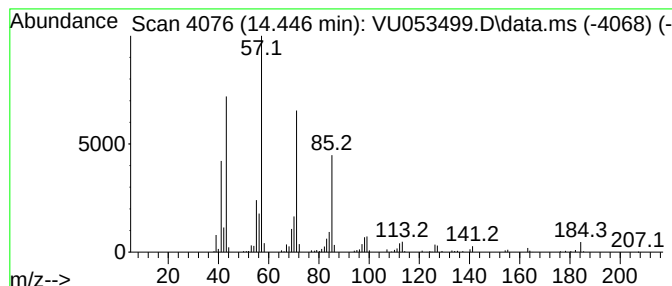
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.446	9.82 ug/L	220403	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	96
2			Tridecane	184	C13H28	000629-50-5	94
3			Tridecane	184	C13H28	000629-50-5	91
4			Dodecane	170	C12H26	000112-40-3	90
5			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033123\
Data File : VU053499.D
Acq On : 31 Mar 2023 18:11
Operator : JC/MD
Sample : 02121-15ME
Misc : 3.42g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C1188ME

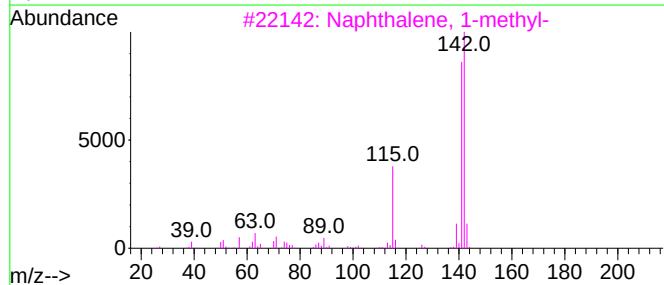
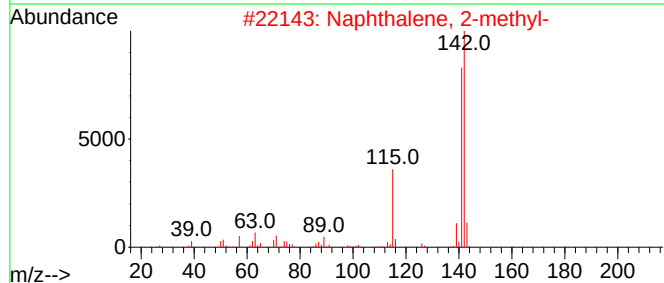
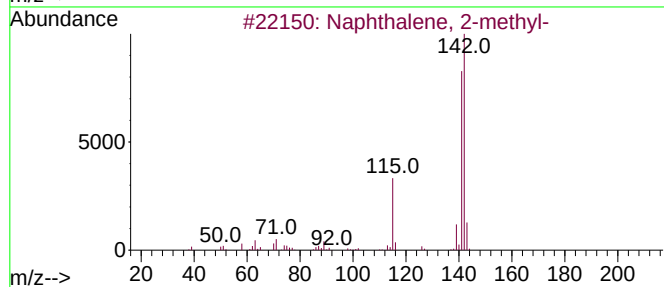
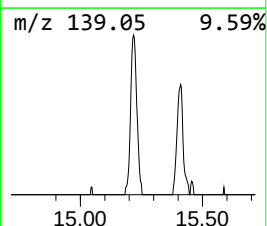
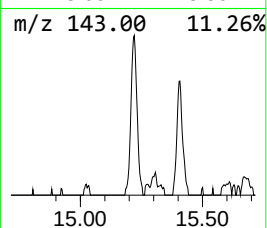
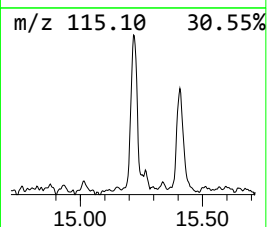
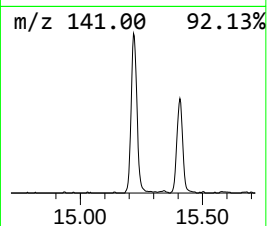
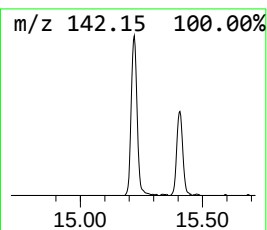
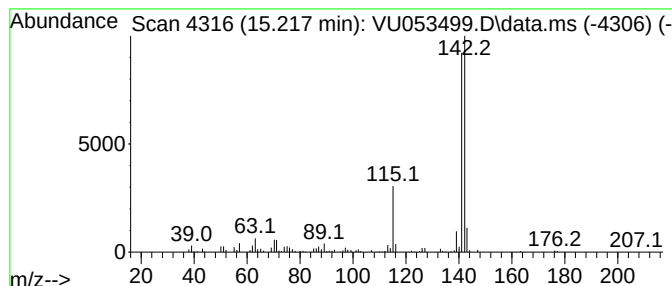
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Quant Title : VOC Analysis

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

Peak Number 7 Naphthalene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.217	6.25 ug/L	140404	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, 2-methyl-	142	C11H10	000091-57-6	96
3			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
4			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	95
5			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033123\
Data File : VU053499.D
Acq On : 31 Mar 2023 18:11
Operator : JC/MD
Sample : 02121-15ME
Misc : 3.42g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C1188ME

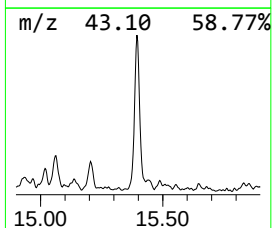
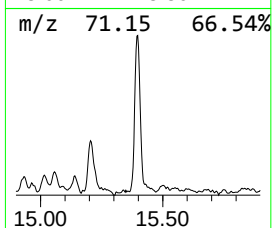
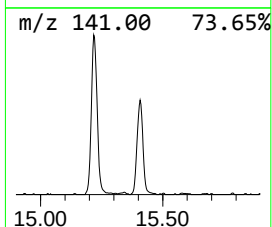
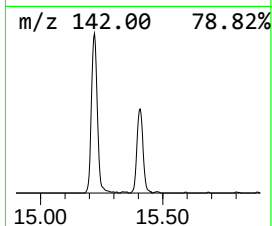
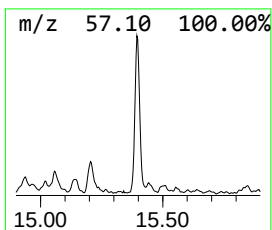
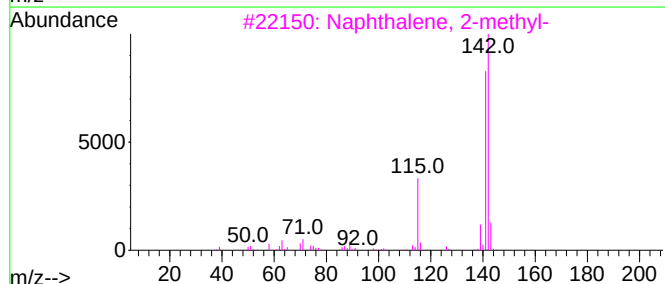
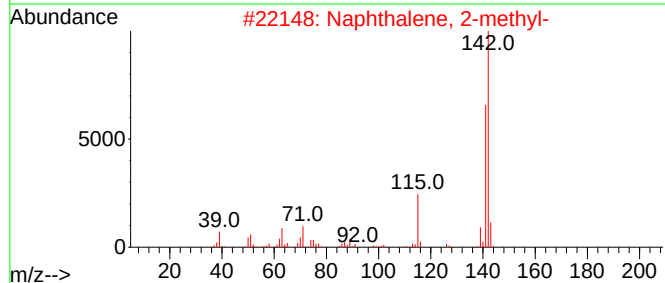
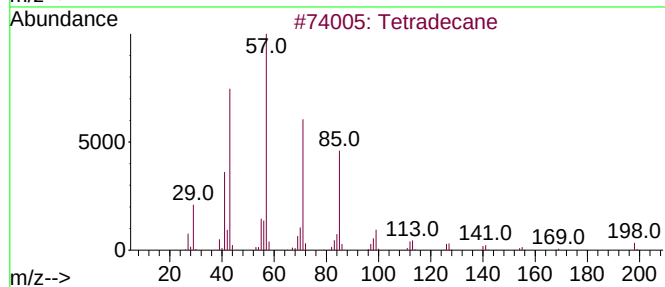
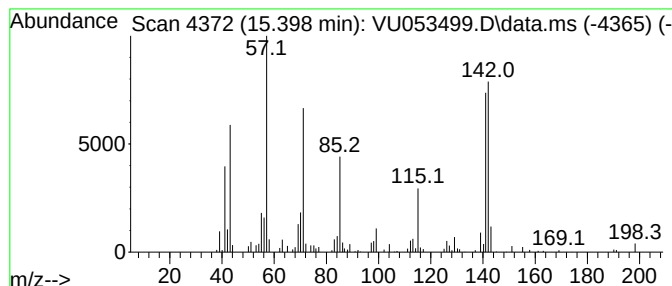
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Quant Title : VOC Analysis

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.398	7.44 ug/L	167049	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	78
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	64
3			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	64
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	60
5			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033123\
Data File : VU053499.D
Acq On : 31 Mar 2023 18:11
Operator : JC/MD
Sample : 02121-15ME
Misc : 3.42g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 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...	12.324	9.3	ug/L	207594	3	11.809	1122520	50.0
(DEL) Alkane: S...	13.427	14.7	ug/L	329683	3	11.809	1122520	50.0
Azulene	14.086	2.8	ug/L	62559	3	11.809	1122520	50.0
Sulfurous acid,...	14.182	3.7	ug/L	82821	3	11.809	1122520	50.0
(DEL) Alkane: S...	14.446	9.8	ug/L	220403	3	11.809	1122520	50.0
Naphthalene, 2-...	15.217	6.3	ug/L	140404	3	11.809	1122520	50.0
(DEL) Alkane: S...	15.398	7.4	ug/L	167049	3	11.809	1122520	50.0