

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042922\
 Data File : VU048355.D
 Acq On : 29 Apr 2022 13:38
 Operator : SY/MD
 Sample : N2562-22ME
 Misc : 7.52g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW481ME

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: VU048355.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	74	80	116	rVB	74517	224909	13.26%	1.631%
2	2.530	357	370	403	rBV	254857	491485	28.98%	3.565%
3	2.748	435	438	449	rVB4	1424	2057	0.12%	0.015%
4	2.803	453	455	460	rVB2	415	326	0.02%	0.002%
5	2.867	470	475	476	rBV3	378	241	0.01%	0.002%
6	2.925	489	493	494	rBV	389	235	0.01%	0.002%
7	2.938	494	497	499	rBV2	501	271	0.02%	0.002%
8	2.954	499	502	503	rBV3	565	341	0.02%	0.002%
9	3.031	515	526	542	rBV3	10100	23830	1.41%	0.173%
10	3.176	558	571	594	rBV	25229	58603	3.46%	0.425%
11	3.665	718	723	724	rVV3	725	632	0.04%	0.005%
12	4.012	828	831	839	rVB	238	259	0.02%	0.002%
13	4.102	854	859	862	rVB2	302	271	0.02%	0.002%
14	4.131	862	868	870	rBV	208	223	0.01%	0.002%
15	4.234	893	900	904	rBV2	202	249	0.01%	0.002%
16	4.449	963	967	970	rBV2	314	223	0.01%	0.002%
17	4.639	1011	1026	1045	rBV	123070	422087	24.89%	3.062%
18	5.064	1141	1158	1187	rBV	266064	662079	39.04%	4.802%
19	5.208	1200	1203	1207	rVB	390	272	0.02%	0.002%
20	5.298	1222	1231	1233	rBV2	609	776	0.05%	0.006%
21	5.443	1273	1276	1281	rVB2	243	214	0.01%	0.002%
22	5.578	1314	1318	1323	rBV2	189	209	0.01%	0.002%
23	5.716	1341	1361	1389	rBV2	671879	1695796	100.00%	12.300%
24	5.935	1424	1429	1430	rBV2	223	196	0.01%	0.001%
25	5.977	1430	1442	1462	rBV4	15304	40016	2.36%	0.290%
26	6.096	1477	1479	1481	rBV2	356	189	0.01%	0.001%
27	6.125	1483	1488	1491	rBV3	488	423	0.02%	0.003%
28	6.176	1491	1504	1510	rBV5	1076	2338	0.14%	0.017%
29	6.247	1511	1526	1554	rVV	463953	960190	56.62%	6.965%
30	6.526	1604	1613	1624	rVV5	5122	10350	0.61%	0.075%
31	6.597	1626	1635	1649	rVV3	6823	15585	0.92%	0.113%
32	6.690	1649	1664	1690	rVB	364995	779771	45.98%	5.656%
33	6.935	1738	1740	1743	rVV	320	210	0.01%	0.002%
34	7.202	1804	1823	1824	rBV3	7539	13311	0.78%	0.097%
35	7.404	1882	1886	1890	rVB2	340	275	0.02%	0.002%
36	7.494	1903	1914	1923	rBV7	1404	2723	0.16%	0.020%

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 ClientSampleId :
 EW481ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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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

37	7.568	1923	1937	1961	rBV	180737	379977	22.41%	2.756%
38	7.684	1968	1973	1974	rBV3	615	446	0.03%	0.003%
39	7.790	1997	2006	2019	rBV4	2729	5419	0.32%	0.039%
40	7.838	2019	2021	2025	rVB3	325	218	0.01%	0.002%
41	7.896	2025	2039	2058	rBV	725541	1382824	81.54%	10.030%
42	8.108	2102	2105	2107	rBV3	499	252	0.01%	0.002%
43	8.124	2107	2110	2116	rVV3	1235	1253	0.07%	0.009%
44	8.182	2116	2128	2155	rVB	112646	260196	15.34%	1.887%
45	8.324	2169	2172	2174	rBV2	321	224	0.01%	0.002%
46	8.353	2174	2181	2183	rBV5	1632	1883	0.11%	0.014%
47	8.536	2232	2238	2242	rBV5	668	635	0.04%	0.005%
48	8.661	2258	2277	2303	rBV	453720	1088644	64.20%	7.896%
49	8.928	2349	2360	2368	rVV6	2991	5354	0.32%	0.039%
50	8.967	2370	2372	2376	rVV2	444	254	0.01%	0.002%
51	8.986	2376	2378	2384	rVB2	490	428	0.03%	0.003%
52	9.028	2385	2391	2393	rBV2	487	435	0.03%	0.003%
53	9.063	2400	2402	2407	rVB2	268	243	0.01%	0.002%
54	9.163	2429	2433	2436	rBV5	1061	986	0.06%	0.007%
55	9.205	2440	2446	2454	rVV5	1716	2306	0.14%	0.017%
56	9.333	2479	2486	2492	rBV3	1464	2035	0.12%	0.015%
57	9.423	2499	2514	2548	rBV	610703	1248053	73.60%	9.053%
58	9.559	2553	2556	2557	rBV2	457	248	0.01%	0.002%
59	9.568	2557	2559	2565	rVB3	735	645	0.04%	0.005%
60	9.655	2581	2586	2589	rBV4	594	611	0.04%	0.004%
61	9.694	2594	2598	2599	rBV2	938	664	0.04%	0.005%
62	9.745	2606	2614	2624	rVB5	3828	6215	0.37%	0.045%
63	9.806	2630	2633	2637	rBV3	444	384	0.02%	0.003%
64	9.874	2647	2654	2658	rVB3	521	524	0.03%	0.004%
65	9.893	2658	2660	2664	rVB	327	201	0.01%	0.001%
66	9.922	2664	2669	2670	rBV	301	277	0.02%	0.002%
67	10.018	2693	2699	2702	rBV5	699	875	0.05%	0.006%
68	10.102	2720	2725	2726	rBV	486	444	0.03%	0.003%
69	10.118	2726	2730	2734	rVB4	937	968	0.06%	0.007%
70	10.247	2763	2770	2779	rVV5	2775	4561	0.27%	0.033%
71	10.346	2798	2801	2802	rBV2	317	195	0.01%	0.001%
72	10.394	2808	2816	2829	rVB4	3085	5754	0.34%	0.042%
73	10.456	2831	2835	2837	rBV3	555	405	0.02%	0.003%
74	10.485	2842	2844	2848	rVV	428	346	0.02%	0.003%
75	10.549	2859	2864	2865	rBV3	756	613	0.04%	0.004%
76	10.594	2874	2878	2880	rBV2	519	409	0.02%	0.003%

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Instrument :
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 ClientSampleId :
 EW481ME

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

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Peak separation: 5

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

77	10.620	2882	2886	2892	rVV6	2424	3464	0.20%	0.025%
78	10.668	2892	2901	2911	rVB6	4016	8030	0.47%	0.058%
79	10.767	2916	2932	2955	rBV	644222	1064143	62.75%	7.719%
80	11.018	3006	3010	3011	rBV3	617	439	0.03%	0.003%
81	11.050	3018	3020	3022	rBV3	454	193	0.01%	0.001%
82	11.066	3022	3025	3028	rVB4	844	457	0.03%	0.003%
83	11.115	3031	3040	3056	rVB2	17048	28767	1.70%	0.209%
84	11.179	3056	3060	3063	rBV4	951	895	0.05%	0.006%
85	11.198	3063	3066	3071	rBV3	583	529	0.03%	0.004%
86	11.311	3094	3101	3109	rBV8	2001	3236	0.19%	0.023%
87	11.417	3127	3134	3142	rBV3	11361	14563	0.86%	0.106%
88	11.462	3142	3148	3167	rVB8	4976	11223	0.66%	0.081%
89	11.574	3176	3183	3190	rBV5	1706	2934	0.17%	0.021%
90	11.693	3215	3220	3231	rBV7	2286	3980	0.23%	0.029%
91	11.816	3245	3258	3273	rBV	777387	1236002	72.89%	8.965%
92	12.002	3303	3316	3324	rVB10	5648	14936	0.88%	0.108%
93	12.198	3359	3377	3395	rBV	800043	1297778	76.53%	9.413%
94	12.327	3409	3417	3429	rBV2	43801	63982	3.77%	0.464%
95	12.902	3591	3596	3598	rBV5	3028	3029	0.18%	0.022%
96	13.047	3636	3641	3650	rVB4	8445	10914	0.64%	0.079%
97	13.134	3662	3668	3677	rVB9	6182	9464	0.56%	0.069%
98	13.433	3751	3761	3770	rBV	57852	87348	5.15%	0.634%
99	13.587	3801	3809	3818	rBV	29133	42055	2.48%	0.305%
100	14.449	4070	4077	4086	rBV	45615	60650	3.58%	0.440%

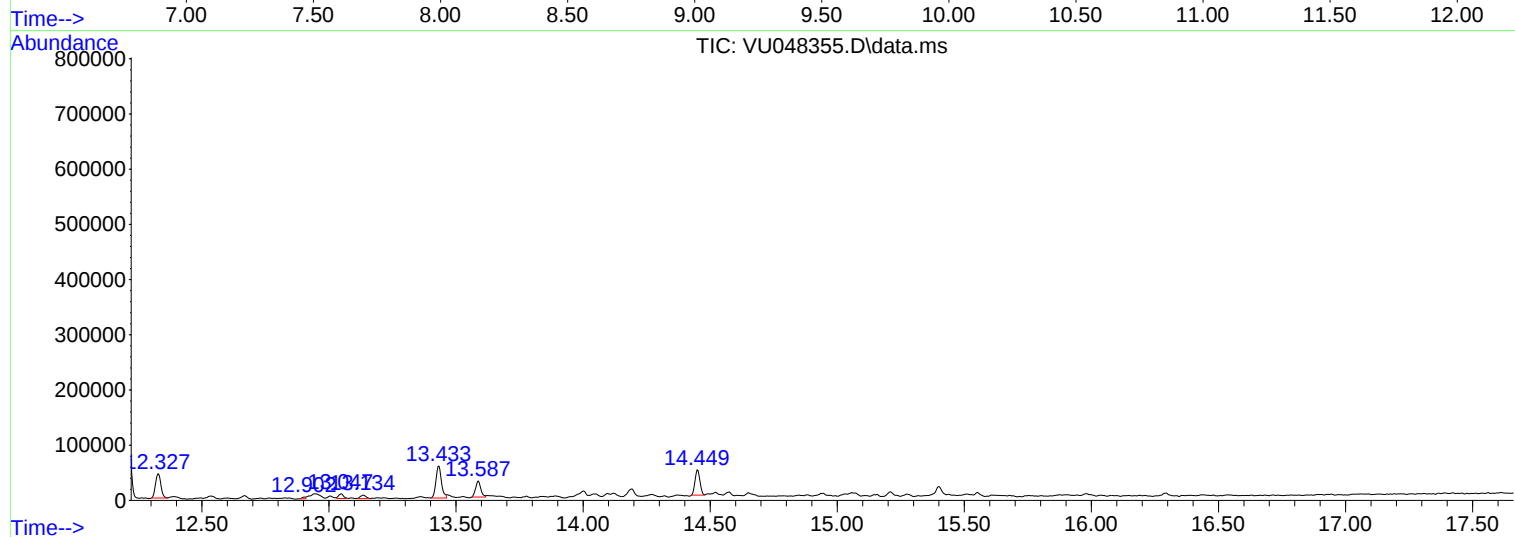
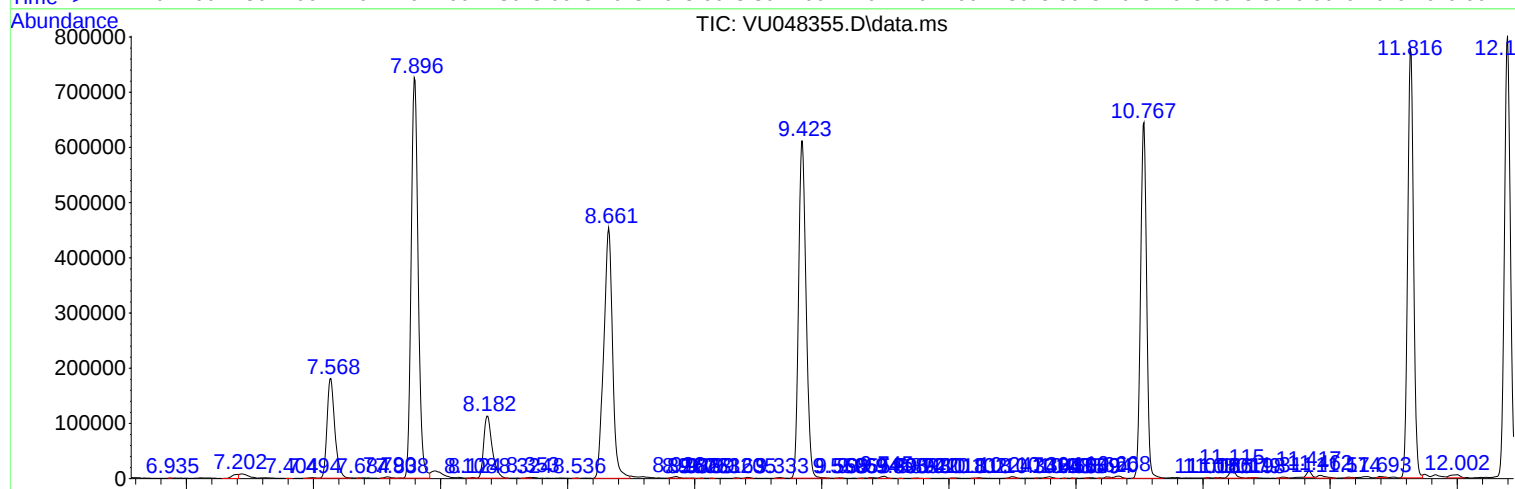
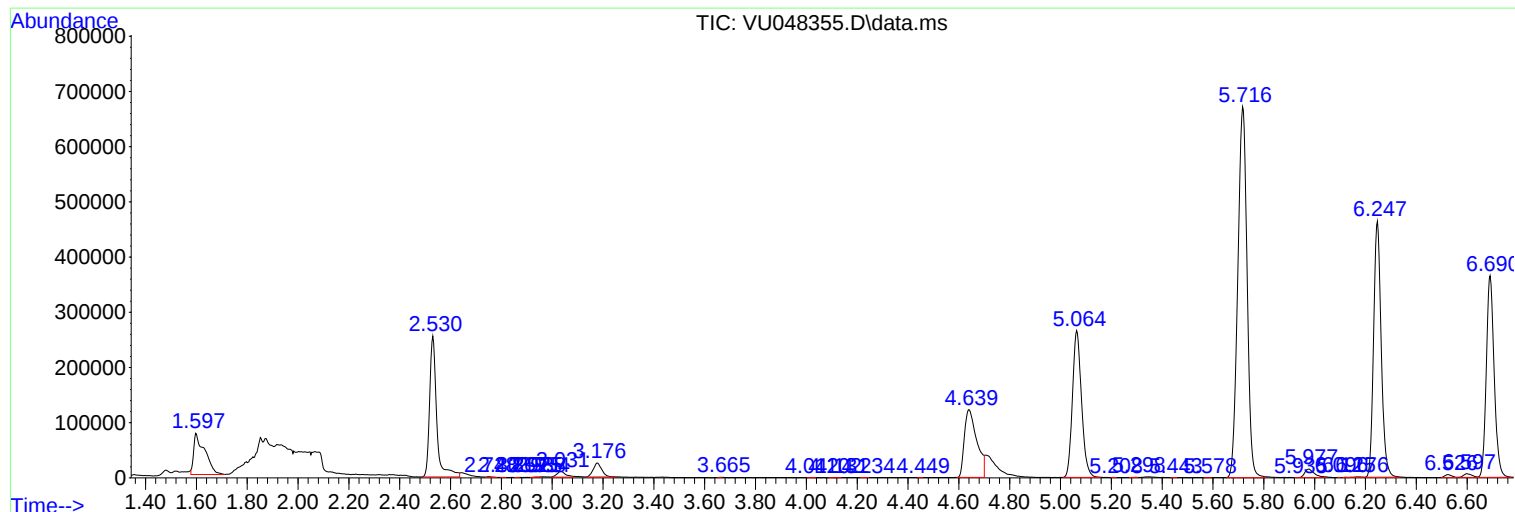
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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW481ME

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 : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW481ME

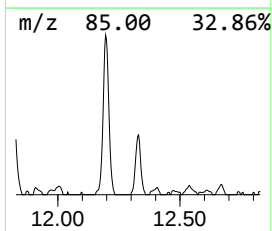
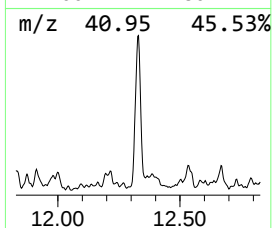
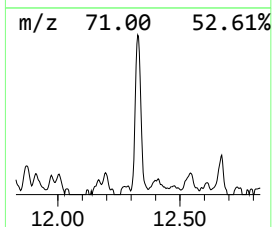
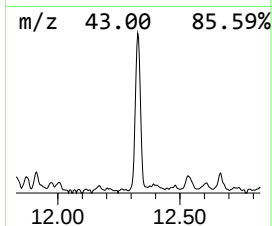
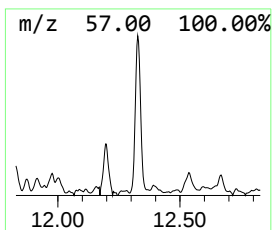
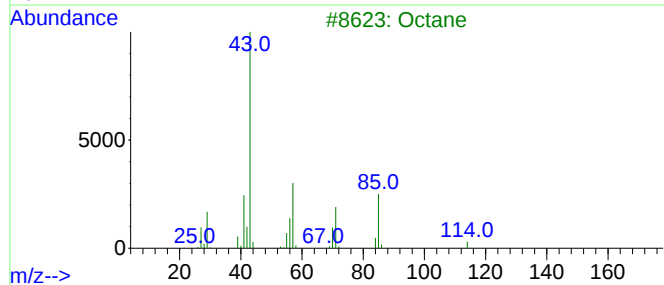
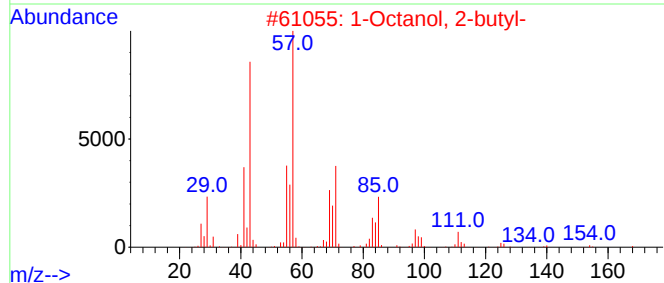
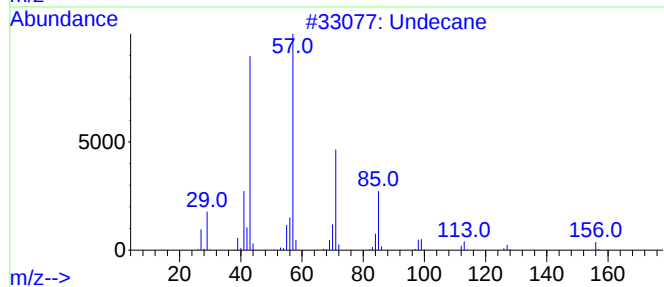
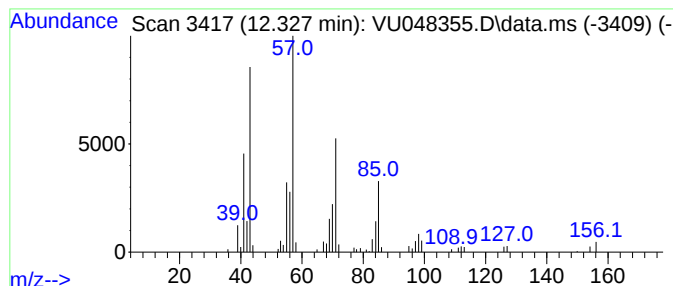
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.327	2.59 ug/L	63982	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane	156	C11H24	001120-21-4	81
2			1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	78
3			Octane	114	C8H18	000111-65-9	72
4			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	72
5			Undecane	156	C11H24	001120-21-4	68



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ALS Vial : 10 Sample Multiplier: 1

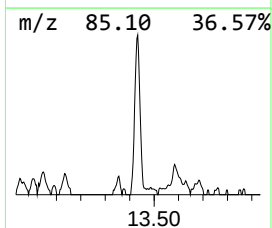
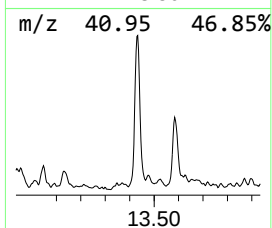
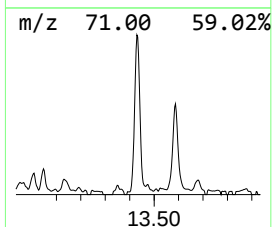
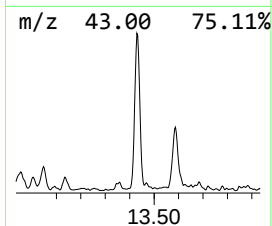
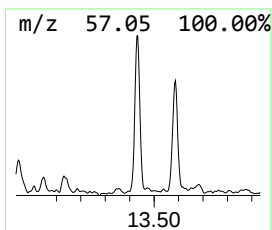
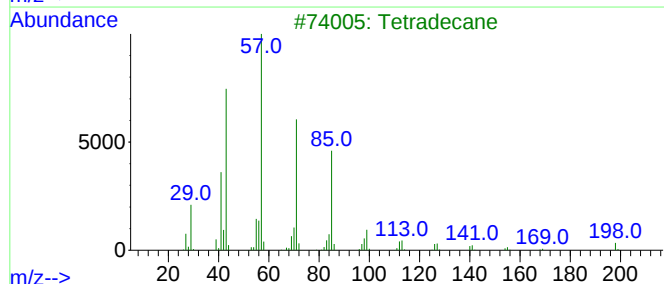
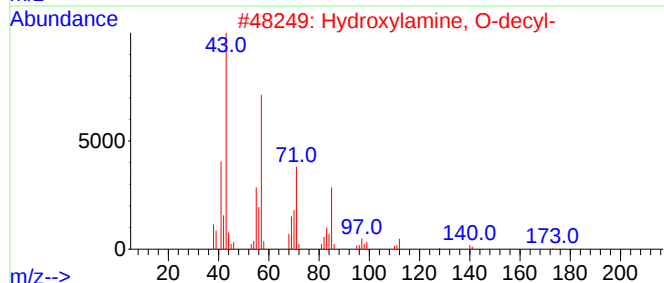
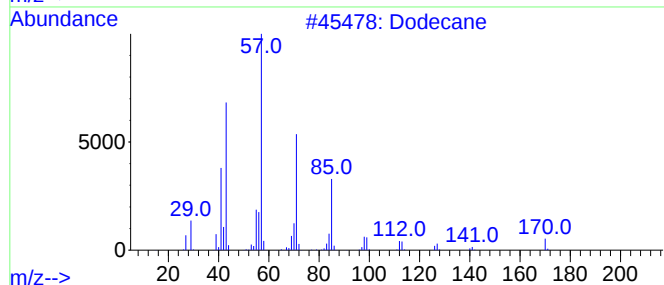
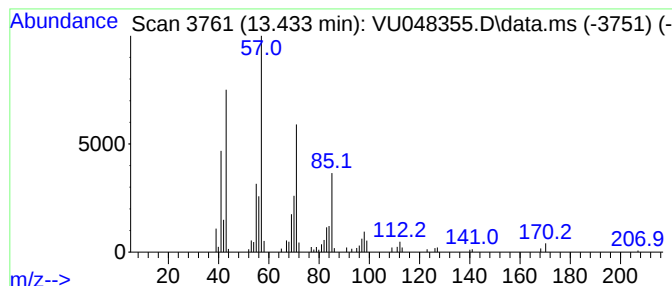
Instrument :
MSVOA_U
ClientSampleId :
EW481ME

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	3.53 ug/L	87348	1,4-Dichlorobenzene-d4		11.816	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Dodecane		170	C12H26	000112-40-3	83
2	Hydroxylamine, O-decyl-		173	C10H23NO	029812-79-1	64
3	Tetradecane		198	C14H30	000629-59-4	53
4	2-Bromo dodecane		248	C12H25Br	013187-99-0	50
5	2-Ethylhexyl mercaptoacetate		204	C10H20O2S	007659-86-1	50



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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	12.327	2.6	ug/L	63982	3	11.816	1236000	50.0
(DEL) Alkane: S...	13.433	3.5	ug/L	87348	3	11.816	1236000	50.0