

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051922\
 Data File : VU048635.D
 Acq On : 19 May 2022 17:17
 Operator : SY/MD
 Sample : N2883-03ME
 Misc : 6.38g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW4K5ME

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\SFAMULM051622WMA.M
 Title : VOC Analysis

Signal : TIC: VU048635.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.594	72	79	104	rBV	39947	77806	8.82%	1.085%
2	2.237	277	279	282	rVB2	421	185	0.02%	0.003%
3	2.385	323	325	329	rVB	458	279	0.03%	0.004%
4	2.536	354	372	384	rBV	151918	247552	28.05%	3.453%
5	2.710	422	426	430	rBB3	439	406	0.05%	0.006%
6	2.764	435	443	453	rVB4	1390	2480	0.28%	0.035%
7	2.951	498	501	503	rBV2	481	340	0.04%	0.005%
8	2.977	508	509	514	rVV3	344	285	0.03%	0.004%
9	3.035	519	527	536	rVB5	1797	3396	0.38%	0.047%
10	3.073	536	539	540	rBV	285	152	0.02%	0.002%
11	3.105	546	549	552	rBV2	238	165	0.02%	0.002%
12	3.182	558	573	589	rBV	15232	37346	4.23%	0.521%
13	3.826	771	773	776	rBB	282	154	0.02%	0.002%
14	3.932	802	806	808	rBV	185	177	0.02%	0.002%
15	4.147	869	873	877	rBB	186	195	0.02%	0.003%
16	4.334	929	931	935	rBB	349	271	0.03%	0.004%
17	4.465	969	972	973	rBB	323	166	0.02%	0.002%
18	4.639	1013	1026	1046	rBV	58118	190274	21.56%	2.654%
19	4.935	1116	1118	1120	rBV	242	169	0.02%	0.002%
20	5.060	1141	1157	1185	rVB	144470	339566	38.47%	4.736%
21	5.350	1239	1247	1251	rBV3	1020	1543	0.17%	0.022%
22	5.581	1316	1319	1323	rVB2	291	225	0.03%	0.003%
23	5.719	1340	1362	1383	rBV2	303284	792134	89.75%	11.049%
24	5.829	1393	1396	1399	rBV	263	194	0.02%	0.003%
25	5.970	1431	1440	1457	rBV4	6973	16683	1.89%	0.233%
26	6.160	1493	1499	1500	rBV	674	416	0.05%	0.006%
27	6.247	1510	1526	1550	rBV	295140	592413	67.12%	8.263%
28	6.423	1579	1581	1585	rVB	294	206	0.02%	0.003%
29	6.526	1602	1613	1622	rBV5	5476	10191	1.15%	0.142%
30	6.597	1625	1635	1649	rVV6	2900	7344	0.83%	0.102%
31	6.690	1649	1664	1687	rVB2	165173	348441	39.48%	4.860%
32	6.774	1687	1690	1693	rBB2	255	162	0.02%	0.002%
33	6.970	1748	1751	1755	rVB2	379	286	0.03%	0.004%
34	7.054	1775	1777	1780	rBB	333	169	0.02%	0.002%
35	7.086	1781	1787	1791	rBV	463	356	0.04%	0.005%
36	7.208	1809	1825	1827	rBV4	5297	10185	1.15%	0.142%

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 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW4K5ME

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\SFAMULM051622WMA.M
 Title : VOC Analysis

37	7.298	1850	1853	1856	rVB2	429	209	0.02%	0.003%
38	7.366	1869	1874	1876	rBV	324	257	0.03%	0.004%
39	7.378	1876	1878	1882	rVB2	260	207	0.02%	0.003%
40	7.443	1896	1898	1901	rBV	253	166	0.02%	0.002%
41	7.494	1910	1914	1916	rBB3	493	320	0.04%	0.004%
42	7.568	1924	1937	1960	rBV	95400	190823	21.62%	2.662%
43	7.793	1995	2007	2015	rBV4	5904	11531	1.31%	0.161%
44	7.896	2027	2039	2056	rBV	351566	637426	72.22%	8.891%
45	8.089	2096	2099	2102	rVB2	379	290	0.03%	0.004%
46	8.112	2103	2106	2107	rBV	304	191	0.02%	0.003%
47	8.118	2107	2108	2111	rVB	525	197	0.02%	0.003%
48	8.182	2115	2128	2151	rBV	64608	135769	15.38%	1.894%
49	8.317	2167	2170	2172	rBV	287	211	0.02%	0.003%
50	8.404	2195	2197	2202	rVB2	230	210	0.02%	0.003%
51	8.436	2204	2207	2210	rBV2	292	232	0.03%	0.003%
52	8.456	2210	2213	2214	rBV2	375	173	0.02%	0.002%
53	8.552	2241	2243	2245	rVB2	470	181	0.02%	0.003%
54	8.587	2250	2254	2256	rVB	274	212	0.02%	0.003%
55	8.661	2259	2277	2299	rBV	198695	473731	53.67%	6.608%
56	8.870	2338	2342	2344	rBV	263	192	0.02%	0.003%
57	8.883	2344	2346	2350	rVB2	266	176	0.02%	0.002%
58	8.928	2350	2360	2364	rBV4	2494	3533	0.40%	0.049%
59	9.060	2399	2401	2405	rVB	452	263	0.03%	0.004%
60	9.153	2426	2430	2432	rBV	309	244	0.03%	0.003%
61	9.211	2445	2448	2449	rBV	447	247	0.03%	0.003%
62	9.275	2466	2468	2474	rVB	211	201	0.02%	0.003%
63	9.314	2474	2480	2483	rBB	293	285	0.03%	0.004%
64	9.366	2494	2496	2499	rVB	271	154	0.02%	0.002%
65	9.420	2500	2513	2539	rBV	380319	756378	85.70%	10.550%
66	9.571	2556	2560	2564	rBV2	548	607	0.07%	0.008%
67	9.687	2592	2596	2597	rBV	645	344	0.04%	0.005%
68	9.745	2607	2614	2620	rBB2	1450	1793	0.20%	0.025%
69	9.854	2641	2648	2653	rBV2	417	515	0.06%	0.007%
70	9.877	2653	2655	2659	rVB2	333	238	0.03%	0.003%
71	9.986	2684	2689	2692	rBV2	311	269	0.03%	0.004%
72	10.050	2707	2709	2715	rVB	249	253	0.03%	0.004%
73	10.092	2716	2722	2725	rBV	325	278	0.03%	0.004%
74	10.121	2725	2731	2737	rVV3	716	857	0.10%	0.012%
75	10.250	2765	2771	2778	rVB3	2914	3352	0.38%	0.047%
76	10.317	2788	2792	2793	rBV	353	251	0.03%	0.004%

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 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW4K5ME

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\SFAMULM051622WMA.M
 Title : VOC Analysis

77	10.398	2809	2817	2825	rVB2	2204	2887	0.33%	0.040%
78	10.558	2859	2867	2869	rBV4	791	752	0.09%	0.010%
79	10.619	2882	2886	2890	rBV3	1559	1547	0.18%	0.022%
80	10.764	2919	2931	2944	rBV	289652	480973	54.50%	6.709%
81	10.841	2953	2955	2958	rVB	368	190	0.02%	0.003%
82	10.864	2958	2962	2963	rBV	331	235	0.03%	0.003%
83	10.896	2966	2972	2977	rVB2	1090	1323	0.15%	0.018%
84	10.964	2990	2993	2995	rBV2	644	333	0.04%	0.005%
85	10.980	2995	2998	2999	rBV	447	249	0.03%	0.003%
86	11.063	3019	3024	3028	rBV4	981	1104	0.13%	0.015%
87	11.115	3033	3040	3058	rVB3	13029	22080	2.50%	0.308%
88	11.192	3059	3064	3073	rVB5	1116	1456	0.16%	0.020%
89	11.230	3073	3076	3079	rBV	468	326	0.04%	0.005%
90	11.298	3094	3097	3098	rBV	482	283	0.03%	0.004%
91	11.353	3112	3114	3116	rBV	417	200	0.02%	0.003%
92	11.536	3168	3171	3173	rBV	232	150	0.02%	0.002%
93	11.745	3233	3236	3237	rBV	1061	638	0.07%	0.009%
94	11.816	3246	3258	3272	rBV	553133	882593	100.00%	12.311%
95	12.070	3335	3337	3339	rBV	321	177	0.02%	0.002%
96	12.198	3365	3377	3391	rVB	453561	724879	82.13%	10.111%
97	12.330	3410	3418	3426	rBV2	27484	38865	4.40%	0.542%
98	12.713	3535	3537	3539	rBV3	1051	615	0.07%	0.009%
99	13.433	3754	3761	3769	rBV2	36421	48923	5.54%	0.682%
100	14.449	4071	4077	4087	rVB2	41237	53506	6.06%	0.746%

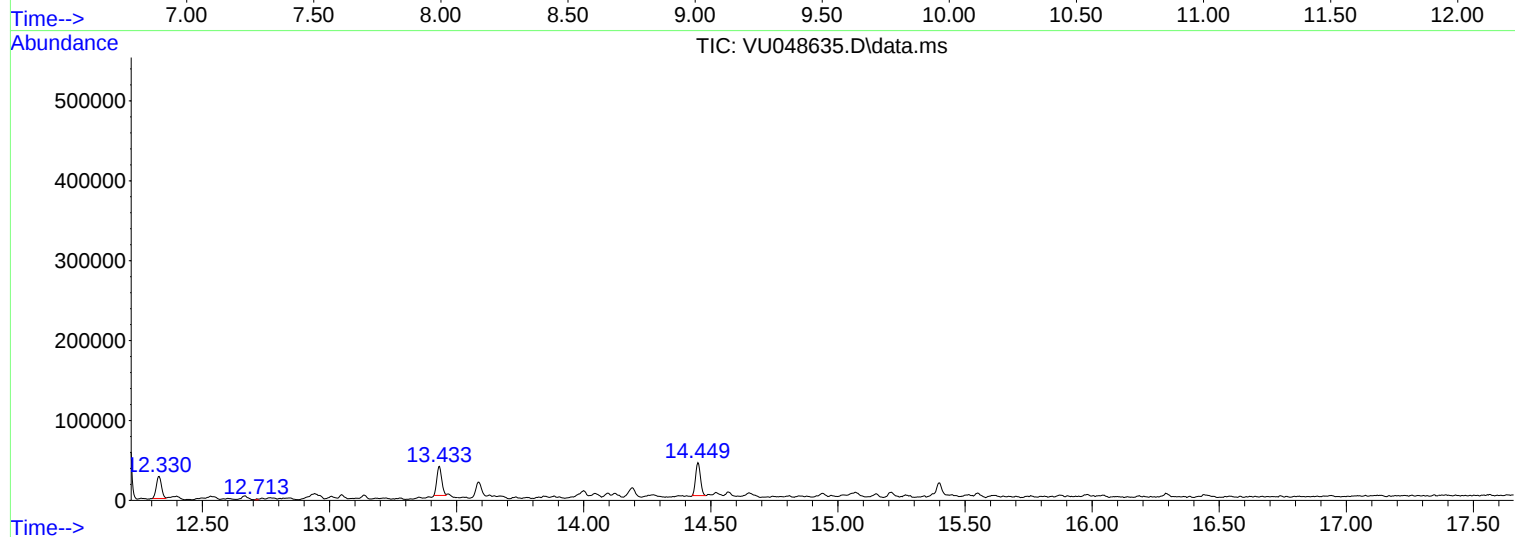
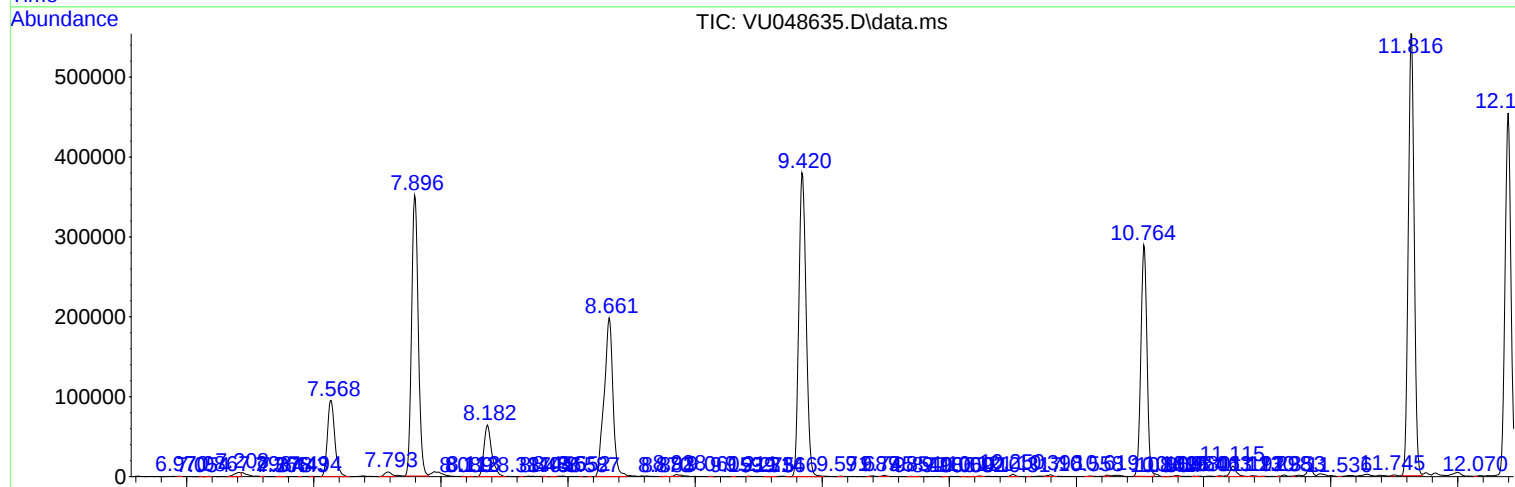
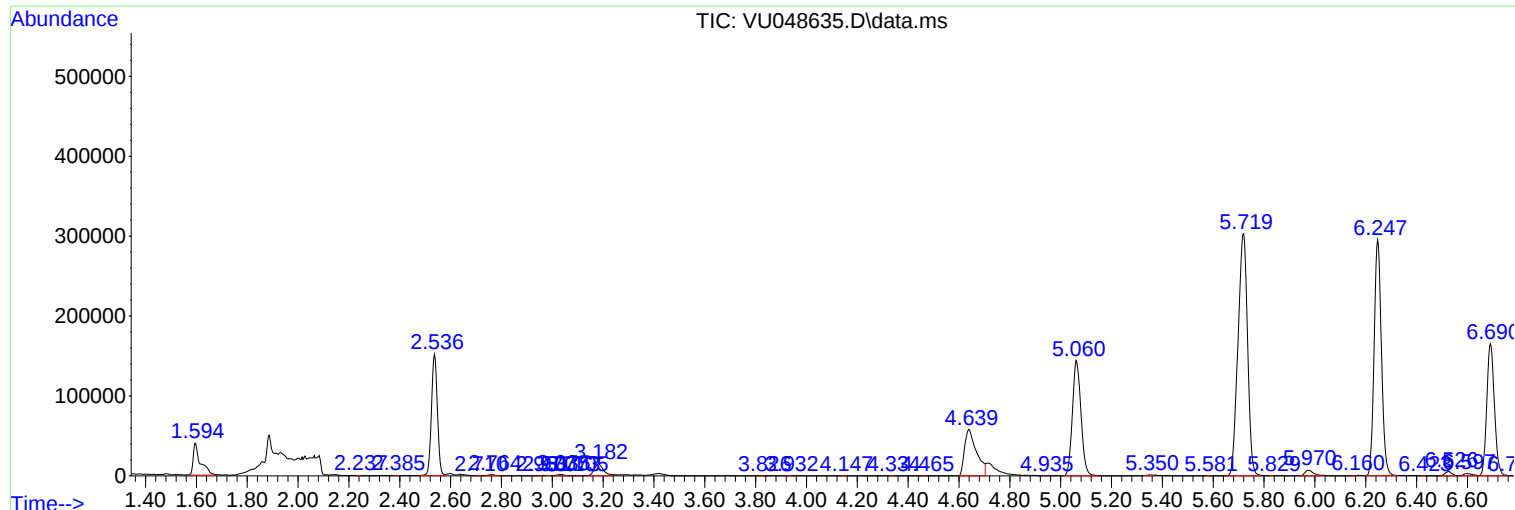
Sum of corrected areas: 7169362

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Misc : 6.38g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4K5ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

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



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Data File : VU048635.D
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Operator : SY/MD
Sample : N2883-03ME
Misc : 6.38g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4K5ME

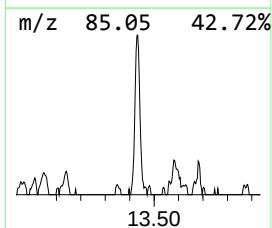
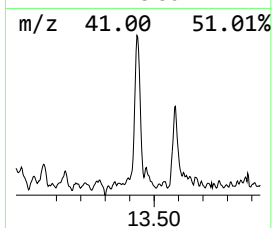
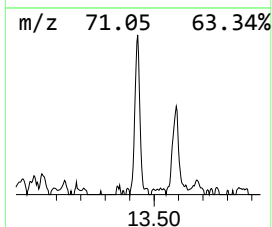
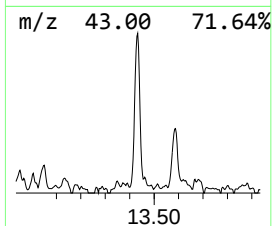
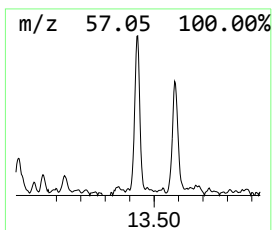
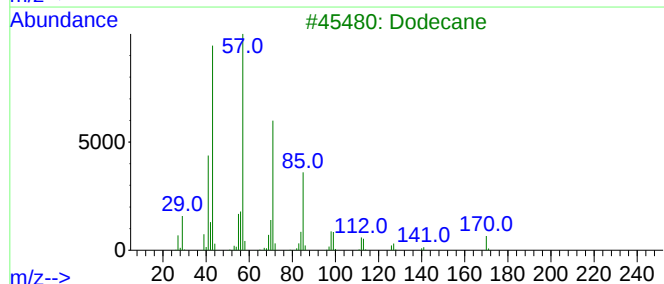
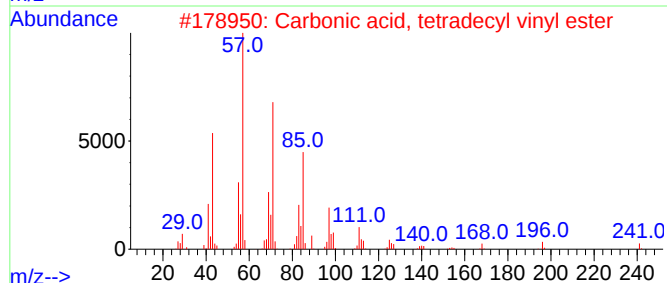
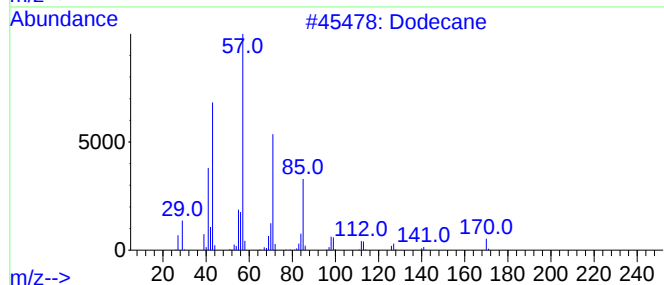
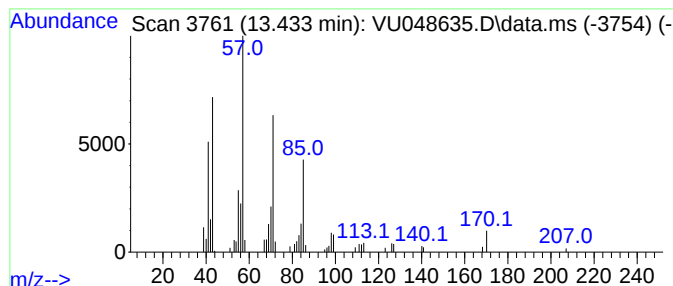
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

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.
13.433	2.77 ug/L	48923	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	94
2			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	80
3			Dodecane	170	C12H26	000112-40-3	74
4			Nonadecane	268	C19H40	000629-92-5	72
5			Tridecane	184	C13H28	000629-50-5	72



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Instrument :
MSVOA_U
ClientSampleId :
EW4K5ME

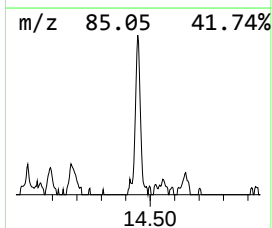
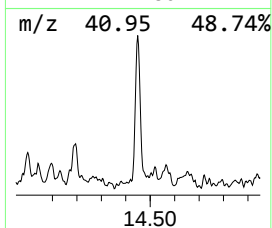
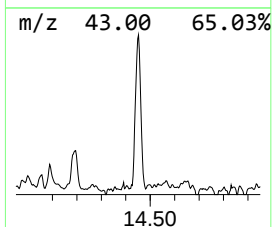
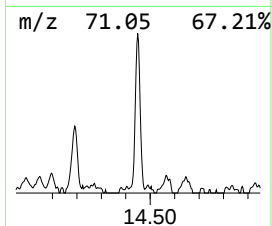
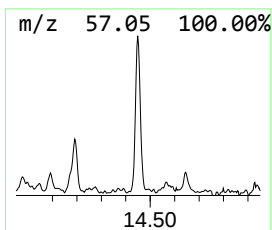
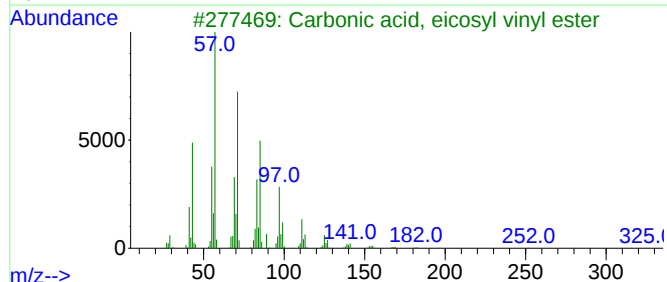
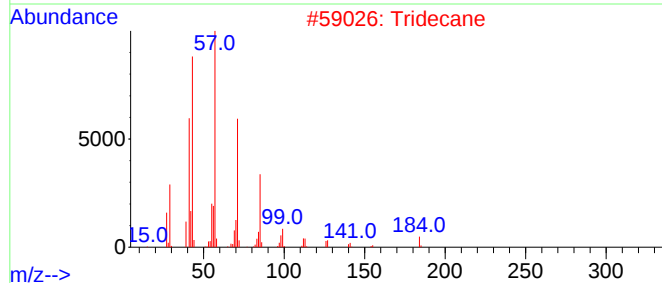
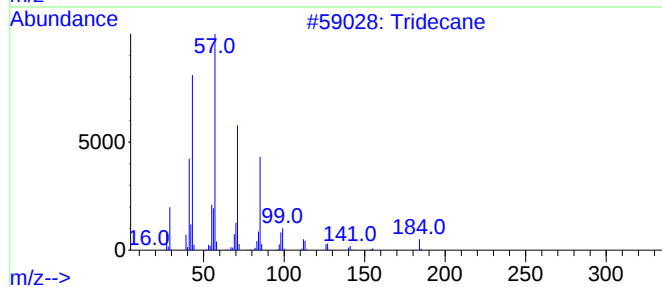
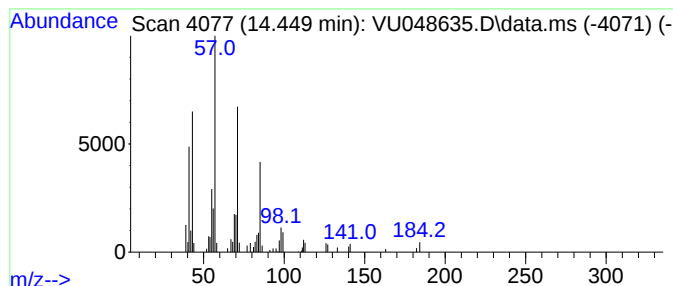
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

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.
14.449	3.03 ug/L	53506	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	96
2			Tridecane	184	C13H28	000629-50-5	93
3			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	86
4			Dodecane	170	C12H26	000112-40-3	86
5			Nonadecane	268	C19H40	000629-92-5	83



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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4K5ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.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...	13.433	2.8	ug/L	48923	3	11.819	882593 50.0
(DEL)	Alkane: S...	14.449	3.0	ug/L	53506	3	11.819	882593 50.0