

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082622\
 Data File : VU050469.D
 Acq On : 26 Aug 2022 20:00
 Operator : SY/MD
 Sample : N4322-07ME
 Misc : 6.04g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EY167ME

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\SFAMULM082422WMA.M
 Title : VOC Analysis

Signal : TIC: VU050469.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.478	38	43	48	rBV3	3930	5014	0.41%	0.048%
2	1.511	49	53	58	rVV4	4136	4674	0.38%	0.045%
3	1.591	71	78	87	rBV	61844	84043	6.81%	0.802%
4	2.520	355	367	384	rVB	185295	301873	24.45%	2.880%
5	3.025	513	524	545	rVB3	10666	22909	1.86%	0.219%
6	3.176	559	571	594	rBV2	19998	53055	4.30%	0.506%
7	3.366	628	630	641	rVB3	896	1039	0.08%	0.010%
8	3.662	717	722	727	rBV3	844	1025	0.08%	0.010%
9	3.800	760	765	768	rBV3	272	237	0.02%	0.002%
10	3.903	793	797	803	rVV2	231	257	0.02%	0.002%
11	4.645	1015	1028	1075	rBV	161718	583341	47.25%	5.565%
12	4.932	1115	1117	1120	rVB4	553	251	0.02%	0.002%
13	5.060	1140	1157	1181	rBV	242616	567376	45.95%	5.413%
14	5.231	1208	1210	1219	rVB3	404	456	0.04%	0.004%
15	5.289	1219	1228	1233	rBV4	1423	2616	0.21%	0.025%
16	5.356	1245	1249	1252	rBV3	470	448	0.04%	0.004%
17	5.575	1315	1317	1323	rVB3	569	399	0.03%	0.004%
18	5.713	1340	1360	1389	rBV2	476181	1234663	100.00%	11.779%
19	5.980	1432	1443	1462	rVV4	11220	27956	2.26%	0.267%
20	6.121	1482	1487	1495	rVB2	1474	1837	0.15%	0.018%
21	6.160	1495	1499	1505	rVB2	280	304	0.02%	0.003%
22	6.243	1508	1525	1553	rBV	356978	718595	58.20%	6.856%
23	6.536	1602	1616	1627	rBV7	9841	20102	1.63%	0.192%
24	6.690	1649	1664	1685	rVB	308391	631176	51.12%	6.022%
25	6.803	1694	1699	1702	rBV5	546	427	0.03%	0.004%
26	6.967	1748	1750	1753	rBV	296	240	0.02%	0.002%
27	7.015	1761	1765	1766	rBV	366	233	0.02%	0.002%
28	7.227	1814	1831	1846	rBV8	5319	13687	1.11%	0.131%
29	7.308	1853	1856	1861	rVB3	592	543	0.04%	0.005%
30	7.494	1907	1914	1920	rBV6	1487	1879	0.15%	0.018%
31	7.565	1920	1936	1955	rBV	126256	244350	19.79%	2.331%
32	7.700	1972	1978	1979	rBV	396	277	0.02%	0.003%
33	7.793	2002	2007	2009	rBV2	425	313	0.03%	0.003%
34	7.896	2026	2039	2059	rBV	370747	674667	54.64%	6.436%
35	7.993	2060	2069	2085	rVB4	6748	16423	1.33%	0.157%
36	8.067	2089	2092	2096	rBV3	798	556	0.05%	0.005%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
 Title : VOC Analysis

37	8.124	2103	2110	2116	rBV5	1742	2571	0.21%	0.025%
38	8.182	2116	2128	2152	rVB	85078	168812	13.67%	1.611%
39	8.317	2167	2170	2175	rBV3	355	322	0.03%	0.003%
40	8.356	2175	2182	2186	rBV5	1241	1768	0.14%	0.017%
41	8.530	2233	2236	2238	rBV3	310	259	0.02%	0.002%
42	8.658	2258	2276	2312	rBV2	491834	1226269	99.32%	11.699%
43	8.861	2336	2339	2345	rVB4	803	782	0.06%	0.007%
44	8.922	2350	2358	2367	rBV6	2927	4947	0.40%	0.047%
45	8.960	2367	2370	2373	rBV4	523	269	0.02%	0.003%
46	9.063	2398	2402	2414	rVB5	880	1290	0.10%	0.012%
47	9.118	2414	2419	2424	rBV2	753	741	0.06%	0.007%
48	9.166	2428	2434	2440	rVV5	1070	1574	0.13%	0.015%
49	9.214	2441	2449	2456	rVB6	1947	3014	0.24%	0.029%
50	9.337	2480	2487	2494	rVB6	2009	2732	0.22%	0.026%
51	9.420	2500	2513	2540	rBV	482369	886584	71.81%	8.458%
52	9.575	2557	2561	2567	rVB4	984	1050	0.09%	0.010%
53	9.652	2582	2585	2586	rBV2	497	322	0.03%	0.003%
54	9.661	2586	2588	2591	rVB2	588	307	0.02%	0.003%
55	9.710	2598	2603	2605	rBV3	700	657	0.05%	0.006%
56	9.726	2606	2608	2609	rVV2	1030	489	0.04%	0.005%
57	9.745	2609	2614	2624	rVB4	2700	3694	0.30%	0.035%
58	9.803	2629	2632	2636	rBV	375	251	0.02%	0.002%
59	9.870	2649	2653	2660	rBV4	665	704	0.06%	0.007%
60	10.021	2693	2700	2712	rVB5	1197	1831	0.15%	0.017%
61	10.115	2723	2729	2733	rBV5	670	722	0.06%	0.007%
62	10.134	2733	2735	2737	rVV	516	267	0.02%	0.003%
63	10.250	2761	2771	2779	rBV4	2688	4754	0.39%	0.045%
64	10.346	2799	2801	2802	rBV2	614	259	0.02%	0.002%
65	10.391	2810	2815	2824	rVB6	3482	5294	0.43%	0.051%
66	10.462	2835	2837	2842	rVB3	557	331	0.03%	0.003%
67	10.558	2859	2867	2873	rBV5	1504	2013	0.16%	0.019%
68	10.623	2879	2887	2893	rBV4	2237	3416	0.28%	0.033%
69	10.764	2917	2931	2957	rVB	671684	1116239	90.41%	10.649%
70	10.909	2974	2976	2981	rVB3	413	259	0.02%	0.002%
71	10.941	2981	2986	2989	rBV2	649	497	0.04%	0.005%
72	11.060	3019	3023	3031	rVV6	1522	2254	0.18%	0.022%
73	11.118	3031	3041	3056	rVV4	8652	14611	1.18%	0.139%
74	11.192	3062	3064	3068	rVV3	639	543	0.04%	0.005%
75	11.250	3079	3082	3087	rBV	496	423	0.03%	0.004%
76	11.317	3096	3103	3111	rBV6	1476	2219	0.18%	0.021%

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Instrument :
 MSVOA_U
 ClientSampleId :
 EY167ME

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\SFAMULM082422WMA.M
 Title : VOC Analysis

77	11.375	3115	3121	3125	rBV3	1330	1502	0.12%	0.014%
78	11.417	3126	3134	3142	rVV4	7788	11188	0.91%	0.107%
79	11.571	3174	3182	3188	rBV6	1299	2113	0.17%	0.020%
80	11.687	3214	3218	3221	rBV3	448	454	0.04%	0.004%
81	11.709	3221	3225	3229	rBV3	987	982	0.08%	0.009%
82	11.742	3232	3235	3242	rVB5	961	1019	0.08%	0.010%
83	11.816	3245	3258	3272	rBV	420764	686669	55.62%	6.551%
84	11.996	3302	3314	3325	rBV	3385	7069	0.57%	0.067%
85	12.105	3346	3348	3355	rVB3	654	491	0.04%	0.005%
86	12.198	3364	3377	3397	rBV	541293	892979	72.33%	8.519%
87	12.327	3408	3417	3428	rBV3	19667	28916	2.34%	0.276%
88	12.481	3462	3465	3467	rBV4	1157	646	0.05%	0.006%
89	12.536	3473	3482	3494	rVB4	3082	6616	0.54%	0.063%
90	12.668	3513	3523	3530	rBV6	4713	7523	0.61%	0.072%
91	12.931	3592	3605	3606	rBV6	3977	5939	0.48%	0.057%
92	13.137	3661	3669	3675	rBV5	3090	4593	0.37%	0.044%
93	13.262	3705	3708	3710	rBV3	1604	1004	0.08%	0.010%
94	13.314	3722	3724	3726	rBV3	752	295	0.02%	0.003%
95	13.433	3751	3761	3781	rBV3	26382	47213	3.82%	0.450%
96	13.533	3786	3792	3795	rBV8	2040	2582	0.21%	0.025%
97	13.587	3801	3809	3819	rBV2	18690	29778	2.41%	0.284%
98	14.449	4070	4077	4085	rBV	24937	33635	2.72%	0.321%
99	15.401	4368	4373	4384	rVB2	13398	17657	1.43%	0.168%
100	15.976	4548	4552	4562	rVB8	6175	8455	0.68%	0.081%

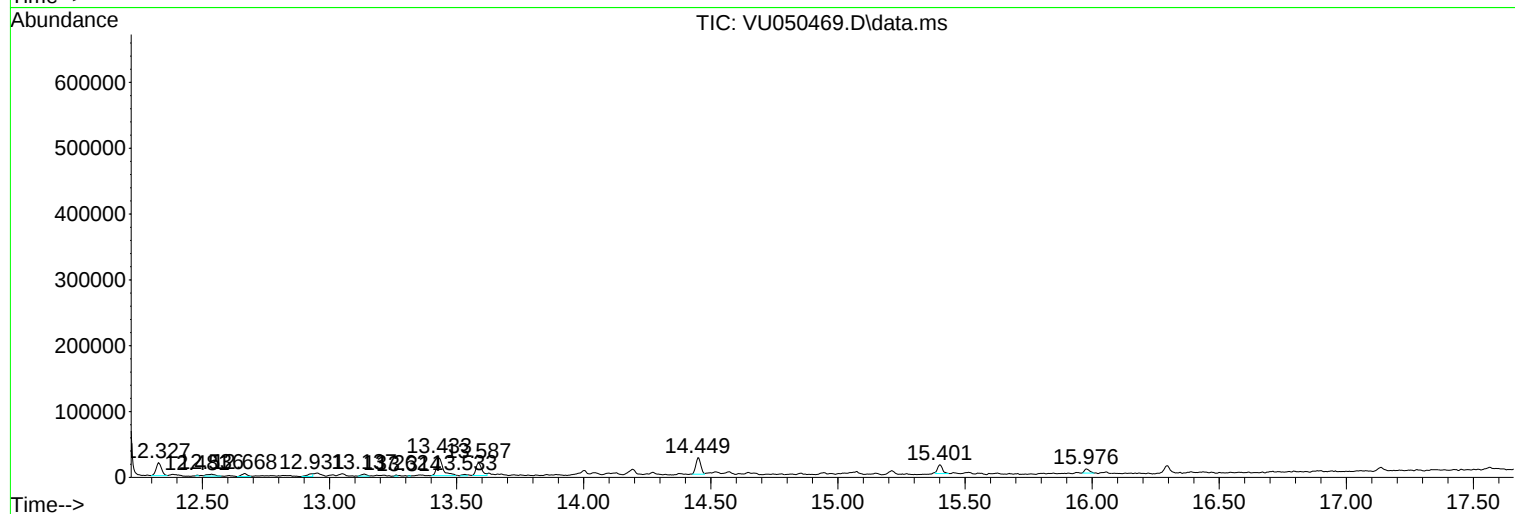
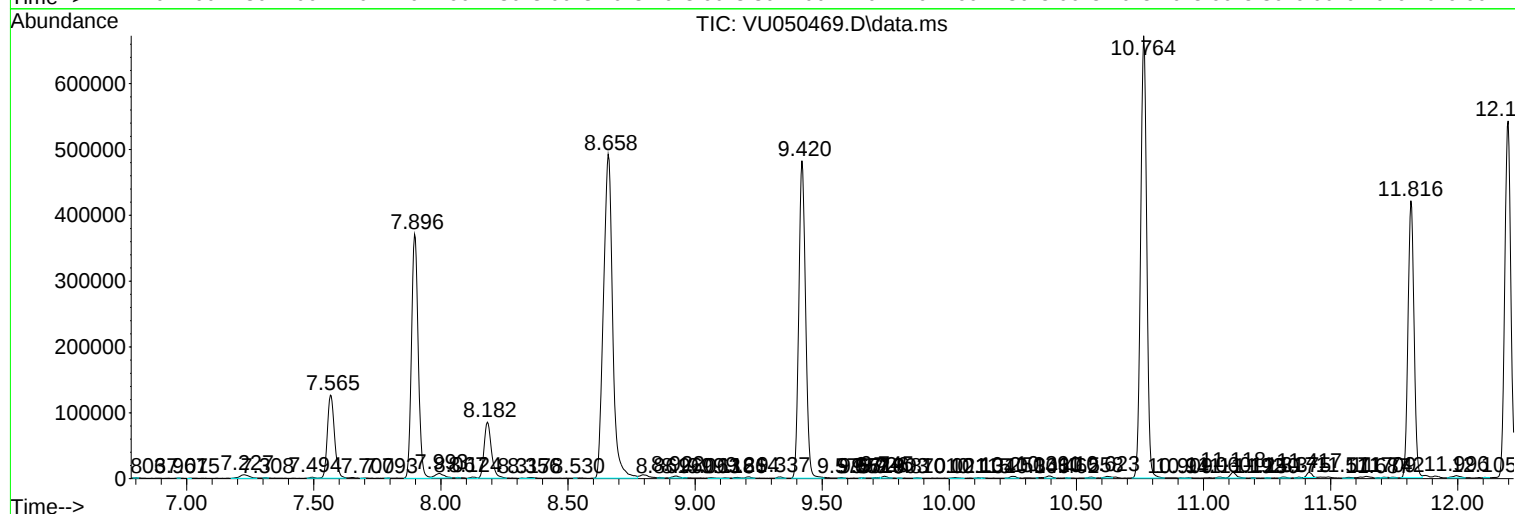
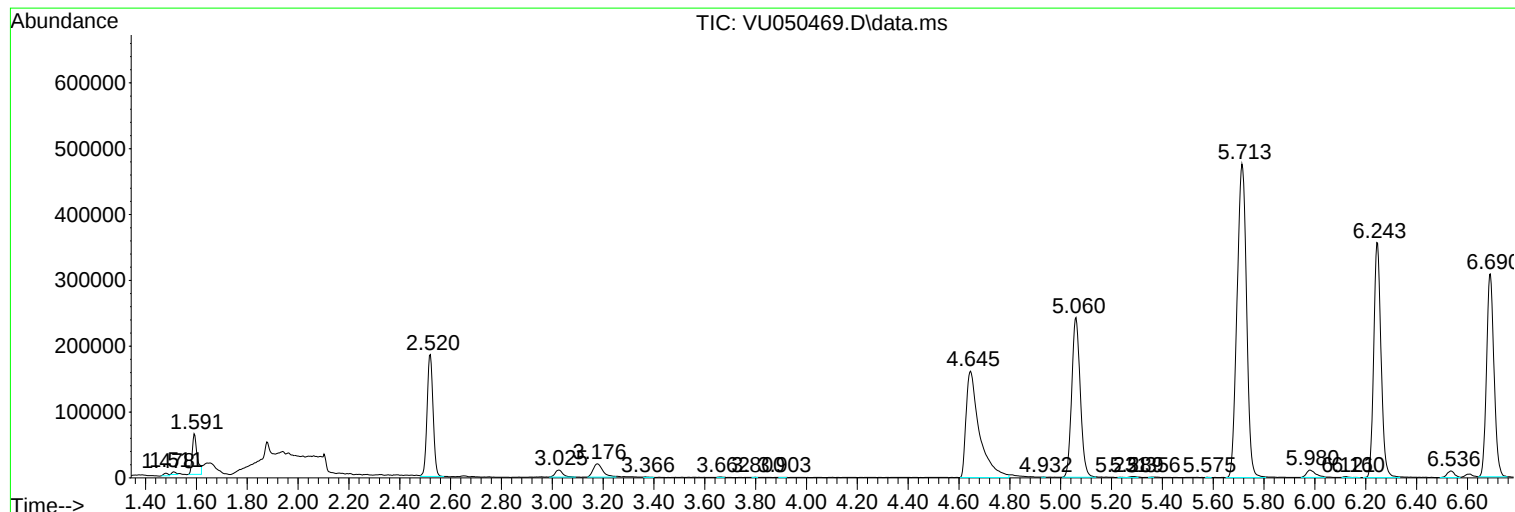
Sum of corrected areas: 10481899

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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY167ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY167ME

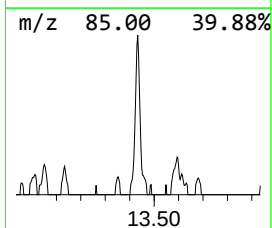
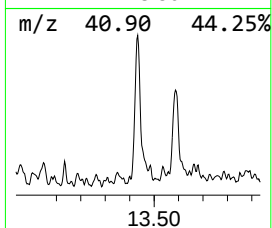
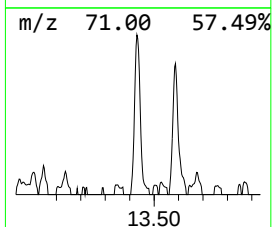
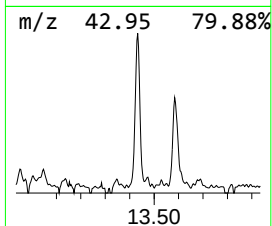
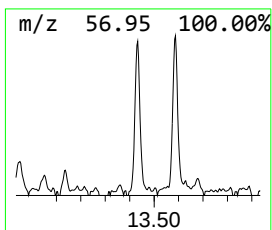
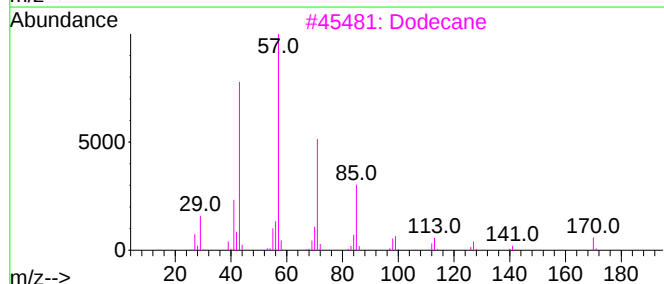
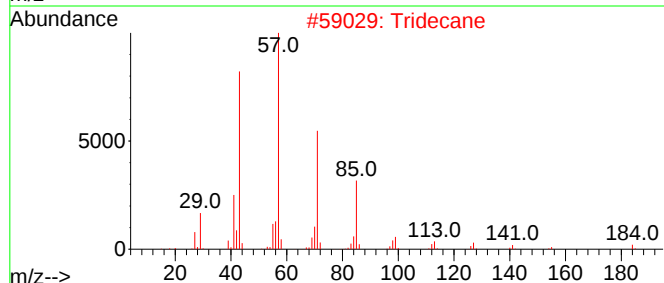
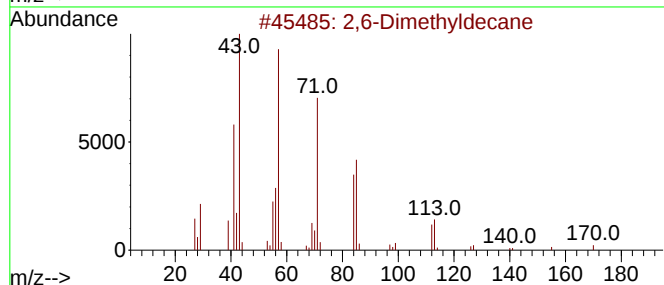
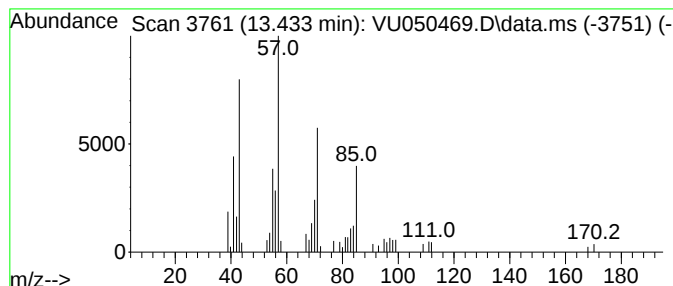
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.433	3.44 ug/L	47213	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,6-Dimethyldecane	170	C12H26	013150-81-7	64
2			Tridecane	184	C13H28	000629-50-5	64
3			Dodecane	170	C12H26	000112-40-3	64
4			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	59
5			Tetradecane	198	C14H30	000629-59-4	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	13.433	3.4	ug/L	47213	3	11.816	686669	50.0