

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV081523\
 Data File : VV031810.D
 Acq On : 15 Aug 2023 14:49
 Operator : SY/MD
 Sample : 03965-07ME
 Misc : 4.09g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 A48H7ME

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_V\Method\SFAMVLM072523WMA.M
 Title : VOC Analysis

Signal : TIC: VV031810.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.275	68	73	92	rVB	118818	175913	10.85%	1.374%
2	2.034	301	309	323	rVB	318604	467620	28.84%	3.653%
3	2.381	410	417	427	rBV	34331	59068	3.64%	0.461%
4	2.793	543	545	546	rBV2	1320	640	0.04%	0.005%
5	2.834	556	558	559	rBV	932	427	0.03%	0.003%
6	2.870	565	569	572	rBV4	1061	937	0.06%	0.007%
7	2.886	572	574	579	rVB5	1972	917	0.06%	0.007%
8	2.915	579	583	588	rBV7	1572	1660	0.10%	0.013%
9	2.976	600	602	603	rBV2	878	348	0.02%	0.003%
10	3.117	644	646	647	rBV2	1429	679	0.04%	0.005%
11	3.162	658	660	663	rBV2	1137	706	0.04%	0.006%
12	3.175	663	664	668	rBV5	956	541	0.03%	0.004%
13	3.217	675	677	678	rBV2	553	154	0.01%	0.001%
14	3.246	684	686	688	rBV3	1424	856	0.05%	0.007%
15	3.391	729	731	733	rBV3	1185	444	0.03%	0.003%
16	3.516	767	770	772	rBV2	1102	743	0.05%	0.006%
17	3.590	791	793	795	rVB3	1485	661	0.04%	0.005%
18	3.600	795	796	798	rVB2	304	117	0.01%	0.001%
19	3.613	798	800	801	rBV2	635	257	0.02%	0.002%
20	3.629	801	805	809	rVB6	921	775	0.05%	0.006%
21	3.706	825	829	830	rBV3	1325	1118	0.07%	0.009%
22	3.741	836	840	843	rBV4	1779	1592	0.10%	0.012%
23	3.809	851	861	895	rBV	119682	421993	26.03%	3.297%
24	4.252	983	999	1034	rBV	274704	754235	46.52%	5.893%
25	4.703	1134	1139	1140	rBV4	1068	732	0.05%	0.006%
26	4.767	1157	1159	1162	rBV4	872	606	0.04%	0.005%
27	4.799	1167	1169	1171	rVB2	932	433	0.03%	0.003%
28	4.850	1184	1185	1187	rBV2	700	312	0.02%	0.002%
29	4.953	1202	1217	1245	rBV2	624353	1621391	100.00%	12.668%
30	5.539	1387	1399	1425	rBV	422615	933289	57.56%	7.292%
31	5.992	1529	1540	1564	rVB	377438	802287	49.48%	6.268%
32	6.294	1631	1634	1635	rBV3	920	492	0.03%	0.004%
33	6.336	1645	1647	1649	rBV3	1549	852	0.05%	0.007%
34	6.503	1697	1699	1701	rVB3	1515	543	0.03%	0.004%
35	6.828	1798	1800	1801	rBV2	1103	379	0.02%	0.003%
36	6.921	1818	1829	1858	rBV	160671	335021	20.66%	2.617%

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 Title : VOC Analysis

37	7.249	1920	1931	1963	rBV	534935	991368	61.14%	7.745%
38	7.561	2019	2028	2052	rBV2	117885	241048	14.87%	1.883%
39	7.979	2156	2158	2159	rBV2	1330	543	0.03%	0.004%
40	8.050	2167	2180	2217	rBV3	354633	989182	61.01%	7.728%
41	8.792	2399	2411	2436	rBV	706231	1248554	77.01%	9.755%
42	9.217	2540	2543	2545	rBV4	1766	1043	0.06%	0.008%
43	9.233	2546	2548	2550	rBV2	1010	525	0.03%	0.004%
44	9.323	2573	2576	2578	rBV3	1750	1081	0.07%	0.008%
45	9.426	2605	2608	2609	rBV3	939	441	0.03%	0.003%
46	9.461	2617	2619	2626	rVB7	1461	1445	0.09%	0.011%
47	9.558	2647	2649	2653	rVB5	1638	832	0.05%	0.007%
48	9.635	2669	2673	2675	rBV4	933	640	0.04%	0.005%
49	9.680	2686	2687	2689	rBV2	846	286	0.02%	0.002%
50	9.693	2689	2691	2692	rBV	967	389	0.02%	0.003%
51	9.702	2692	2694	2698	rVB4	1263	827	0.05%	0.006%
52	9.725	2698	2701	2707	rVB6	1554	1102	0.07%	0.009%
53	9.751	2707	2709	2714	rVB3	1197	985	0.06%	0.008%
54	9.776	2714	2717	2718	rBV3	1650	929	0.06%	0.007%
55	9.815	2726	2729	2733	rVB5	1214	995	0.06%	0.008%
56	9.966	2774	2776	2778	rBV3	1323	594	0.04%	0.005%
57	10.014	2789	2791	2793	rVB2	1028	434	0.03%	0.003%
58	10.037	2795	2798	2802	rBV5	1156	1035	0.06%	0.008%
59	10.056	2802	2804	2809	rVB6	1122	842	0.05%	0.007%
60	10.082	2810	2812	2817	rVB5	1366	912	0.06%	0.007%
61	10.104	2817	2819	2821	rBV4	533	263	0.02%	0.002%
62	10.124	2821	2825	2826	rBV3	1937	1294	0.08%	0.010%
63	10.162	2826	2837	2860	rVV	593196	995005	61.37%	7.774%
64	10.400	2910	2911	2915	rVB4	1299	552	0.03%	0.004%
65	10.423	2915	2918	2922	rBV4	1434	794	0.05%	0.006%
66	10.477	2933	2935	2936	rBV2	759	274	0.02%	0.002%
67	10.664	2991	2993	2994	rBV2	824	395	0.02%	0.003%
68	10.734	3013	3015	3016	rBV3	947	265	0.02%	0.002%
69	10.815	3031	3040	3053	rBV4	13146	26376	1.63%	0.206%
70	10.976	3088	3090	3091	rBV2	1352	544	0.03%	0.004%
71	11.194	3147	3158	3177	rBV	831705	1284041	79.19%	10.032%
72	11.474	3242	3245	3250	rBV5	1658	1116	0.07%	0.009%
73	11.496	3250	3252	3258	rBV7	1125	1282	0.08%	0.010%
74	11.567	3263	3274	3297	rBV	789250	1258162	77.60%	9.830%
75	12.066	3426	3429	3430	rBV3	1376	642	0.04%	0.005%
76	12.168	3459	3461	3463	rBV3	1205	635	0.04%	0.005%

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Title : VOC Analysis

77	12.181	3463	3465	3466	rBV3	1536	622	0.04%	0.005%
78	12.480	3555	3558	3559	rBV3	1473	780	0.05%	0.006%
79	12.551	3577	3580	3583	rVB5	996	757	0.05%	0.006%
80	12.580	3583	3589	3590	rBV6	1622	1615	0.10%	0.013%
81	12.815	3659	3662	3664	rBV3	1433	948	0.06%	0.007%
82	12.860	3674	3676	3680	rVB5	1491	1082	0.07%	0.008%
83	12.882	3680	3683	3686	rBV5	838	672	0.04%	0.005%
84	12.911	3686	3692	3693	rBV4	1437	1362	0.08%	0.011%
85	13.021	3718	3726	3736	rBV3	14836	24532	1.51%	0.192%
86	13.316	3816	3818	3821	rBV3	1283	628	0.04%	0.005%
87	14.365	4128	4144	4161	rBV	62434	120151	7.41%	0.939%

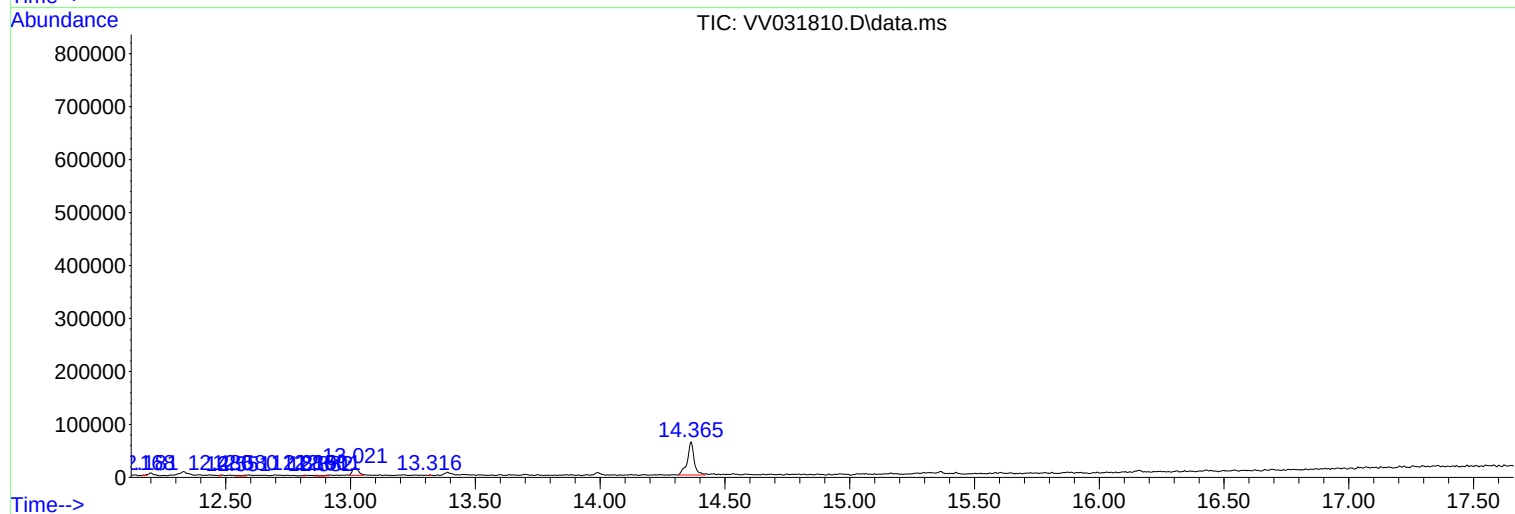
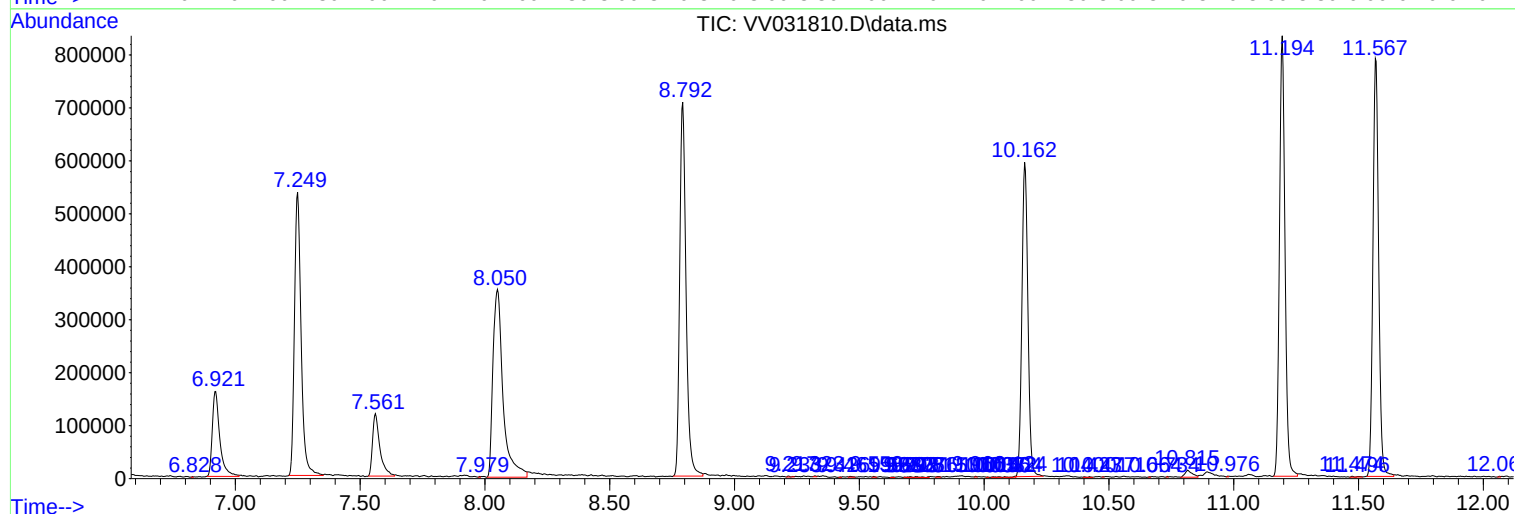
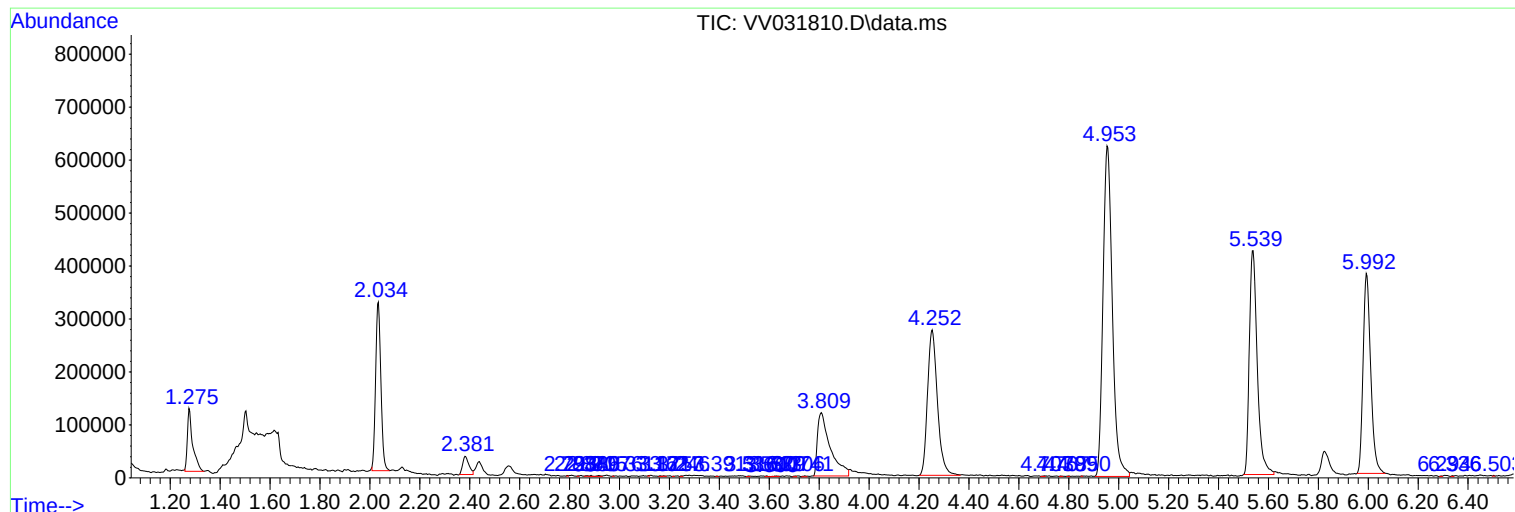
Sum of corrected areas: 12799559

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

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



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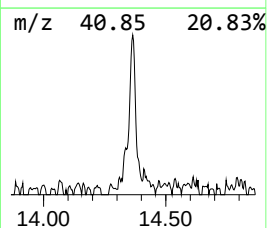
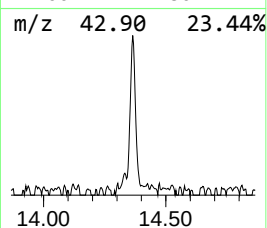
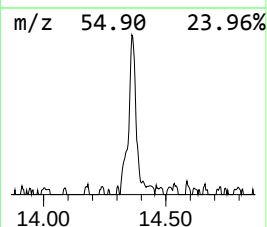
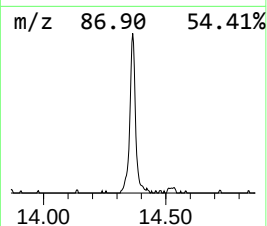
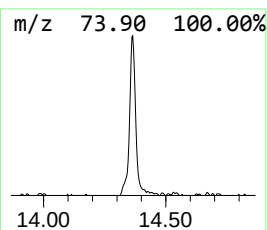
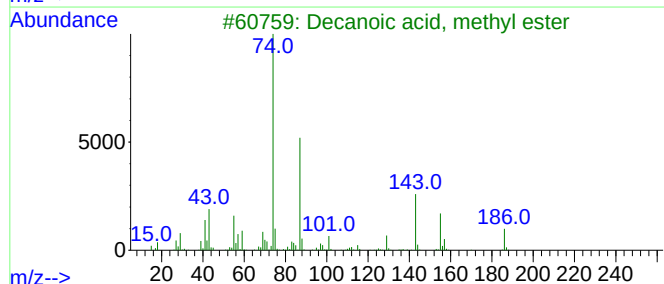
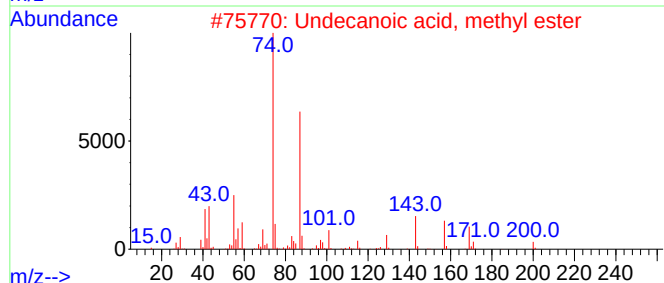
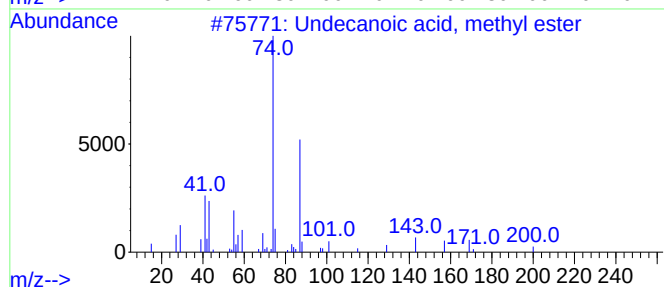
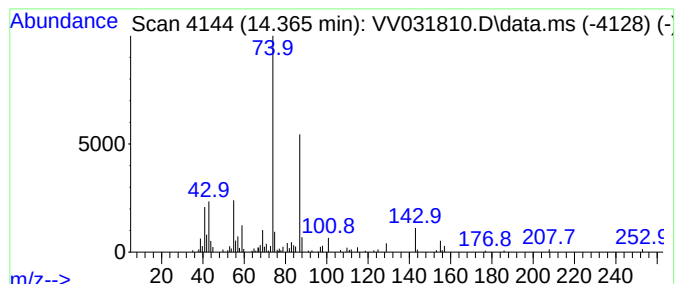
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Undecanoic acid, methyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.365	4.68 ug/L	120151	1,4-Dichlorobenzene-d4	11.194

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecanoic acid, methyl ester	200	C12H24O2	001731-86-8	90
2			Undecanoic acid, methyl ester	200	C12H24O2	001731-86-8	86
3			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	83
4			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	83
5			Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	78



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Undecanoic acid...	14.365	4.7	ug/L	120151	3	11.194	1284040	50.0