

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050222\
 Data File : VU048379.D
 Acq On : 02 May 2022 20:42
 Operator : SY/MD
 Sample : N2638-09ME
 Misc : 4.94g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXL04ME

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: VU048379.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.482	37	44	52	rBV	38290	49145	3.29%	0.380%
2	1.601	73	81	100	rBV	107749	161124	10.80%	1.246%
3	1.874	162	166	197	rVB	93951	159098	10.66%	1.230%
4	2.556	365	378	396	rVV	256713	426428	28.57%	3.297%
5	2.636	396	403	414	rVB2	8485	15269	1.02%	0.118%
6	2.791	442	451	454	rBV3	1129	1415	0.09%	0.011%
7	2.810	454	457	463	rBV3	1087	1188	0.08%	0.009%
8	2.897	481	484	490	rVB4	556	506	0.03%	0.004%
9	2.929	490	494	496	rBV2	714	494	0.03%	0.004%
10	2.951	496	501	510	rVB5	1301	1745	0.12%	0.013%
11	3.045	520	530	533	rBV5	3044	4939	0.33%	0.038%
12	3.180	556	572	591	rBV	64385	152909	10.25%	1.182%
13	3.331	615	619	622	rVV2	711	601	0.04%	0.005%
14	3.360	622	628	631	rVB3	386	425	0.03%	0.003%
15	3.395	635	639	642	rBV2	875	687	0.05%	0.005%
16	3.582	693	697	700	rBV	750	532	0.04%	0.004%
17	3.758	749	752	759	rBV2	675	670	0.04%	0.005%
18	3.800	759	765	768	rVV	690	572	0.04%	0.004%
19	3.826	768	773	777	rVV2	535	527	0.04%	0.004%
20	3.919	799	802	806	rVV	672	437	0.03%	0.003%
21	4.135	864	869	874	rBV	753	727	0.05%	0.006%
22	4.167	874	879	882	rBV	544	510	0.03%	0.004%
23	4.215	892	894	897	rBV	749	492	0.03%	0.004%
24	4.250	902	905	910	rVB2	453	434	0.03%	0.003%
25	4.324	922	928	932	rBV2	567	650	0.04%	0.005%
26	4.623	1005	1021	1040	rBV	174261	448880	30.08%	3.471%
27	4.855	1091	1093	1095	rVB	978	428	0.03%	0.003%
28	4.893	1102	1105	1108	rVB	848	617	0.04%	0.005%
29	4.938	1114	1119	1121	rBV2	636	534	0.04%	0.004%
30	5.061	1142	1157	1180	rVV	277150	603183	40.41%	4.664%
31	5.202	1191	1201	1214	rBV2	5425	10597	0.71%	0.082%
32	5.273	1219	1223	1226	rBV	998	856	0.06%	0.007%
33	5.308	1231	1234	1236	rBV4	692	485	0.03%	0.004%
34	5.327	1237	1240	1241	rBV2	1156	622	0.04%	0.005%
35	5.434	1267	1273	1279	rBV	821	1074	0.07%	0.008%
36	5.540	1303	1306	1314	rVB	506	495	0.03%	0.004%

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Integrator: RTE

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

37	5.723	1341	1363	1384	rBV2	558210	1492497	100.00%	11.540%
38	5.945	1428	1432	1433	rBV	720	554	0.04%	0.004%
39	5.967	1433	1439	1453	rVB6	3500	6948	0.47%	0.054%
40	6.089	1471	1477	1479	rBV2	497	520	0.03%	0.004%
41	6.109	1479	1483	1485	rBV	585	449	0.03%	0.003%
42	6.160	1492	1499	1500	rBV4	1664	1807	0.12%	0.014%
43	6.247	1512	1526	1546	rBV	503107	943176	63.19%	7.293%
44	6.395	1564	1572	1581	rBV6	5164	9214	0.62%	0.071%
45	6.520	1607	1611	1613	rBV2	1692	1428	0.10%	0.011%
46	6.604	1629	1637	1645	rVB6	2642	4753	0.32%	0.037%
47	6.691	1648	1664	1683	rBV	353751	693975	46.50%	5.366%
48	6.925	1731	1737	1750	rVB3	4422	8368	0.56%	0.065%
49	7.183	1808	1817	1833	rVB7	12971	27505	1.84%	0.213%
50	7.405	1881	1886	1892	rBV3	739	1124	0.08%	0.009%
51	7.466	1902	1905	1910	rBV	556	580	0.04%	0.004%
52	7.565	1924	1936	1955	rVV	187418	326531	21.88%	2.525%
53	7.687	1969	1974	1975	rBV3	1155	865	0.06%	0.007%
54	7.784	1999	2004	2006	rBV4	2547	2444	0.16%	0.019%
55	7.896	2021	2039	2056	rBV	673011	1174079	78.67%	9.078%
56	8.128	2108	2111	2114	rBV	617	435	0.03%	0.003%
57	8.179	2115	2127	2143	rBV	137148	231910	15.54%	1.793%
58	8.276	2154	2157	2160	rBV2	844	538	0.04%	0.004%
59	8.552	2233	2243	2256	rVB2	28725	48638	3.26%	0.376%
60	8.639	2256	2270	2301	rBV	570605	1084522	72.66%	8.385%
61	8.893	2345	2349	2355	rBV2	577	525	0.04%	0.004%
62	9.093	2407	2411	2414	rVB2	624	489	0.03%	0.004%
63	9.154	2427	2430	2435	rBV3	628	542	0.04%	0.004%
64	9.311	2476	2479	2483	rBV	697	739	0.05%	0.006%
65	9.417	2498	2512	2543	rBV	729408	1230930	82.47%	9.517%
66	9.694	2594	2598	2607	rVB2	1341	1461	0.10%	0.011%
67	9.829	2634	2640	2641	rBV	723	588	0.04%	0.005%
68	9.858	2646	2649	2653	rBV2	673	681	0.05%	0.005%
69	9.919	2665	2668	2671	rBV	564	476	0.03%	0.004%
70	10.054	2706	2710	2716	rBV	548	671	0.04%	0.005%
71	10.189	2748	2752	2758	rBV3	666	702	0.05%	0.005%
72	10.269	2775	2777	2784	rVB2	699	575	0.04%	0.004%
73	10.404	2816	2819	2829	rVB2	783	1070	0.07%	0.008%
74	10.517	2849	2854	2857	rBV2	541	516	0.03%	0.004%
75	10.665	2896	2900	2910	rVB3	1958	2541	0.17%	0.020%
76	10.758	2917	2929	2948	rVV	652512	1059916	71.02%	8.195%

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 ALS Vial : 23 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
 EXL04ME

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

77	10.855	2955	2959	2962	rBV2	869	699	0.05%	0.005%
78	11.057	3016	3022	3028	rVB4	1618	1935	0.13%	0.015%
79	11.115	3031	3040	3049	rVV2	26483	37723	2.53%	0.292%
80	11.298	3094	3097	3101	rVB2	724	535	0.04%	0.004%
81	11.321	3101	3104	3109	rBV	731	633	0.04%	0.005%
82	11.681	3213	3216	3218	rBV2	663	474	0.03%	0.004%
83	11.700	3218	3222	3226	rVV3	985	1031	0.07%	0.008%
84	11.813	3245	3257	3273	rBV	787194	1228579	82.32%	9.499%
85	11.912	3284	3288	3297	rVB9	1682	2145	0.14%	0.017%
86	11.970	3304	3306	3311	rVB3	1375	912	0.06%	0.007%
87	12.195	3362	3376	3396	rBV	742598	1220159	81.75%	9.434%
88	12.327	3411	3417	3427	rVB2	6978	9397	0.63%	0.073%
89	12.533	3474	3481	3485	rBV3	906	1288	0.09%	0.010%
90	12.684	3523	3528	3529	rBV	806	646	0.04%	0.005%
91	12.845	3574	3578	3580	rBV2	845	647	0.04%	0.005%
92	12.883	3588	3590	3596	rVB2	819	633	0.04%	0.005%
93	13.073	3645	3649	3654	rBV2	543	635	0.04%	0.005%
94	13.141	3667	3670	3672	rBV3	681	514	0.03%	0.004%
95	13.391	3743	3748	3755	rBV6	2568	3631	0.24%	0.028%
96	13.430	3755	3760	3768	rVV5	1542	2169	0.15%	0.017%
97	13.581	3804	3807	3808	rBV2	714	461	0.03%	0.004%
98	13.825	3879	3883	3885	rBV2	624	561	0.04%	0.004%
99	14.182	3991	3994	4001	rVB4	1438	1577	0.11%	0.012%
100	14.446	4071	4076	4080	rBV5	1345	1851	0.12%	0.014%

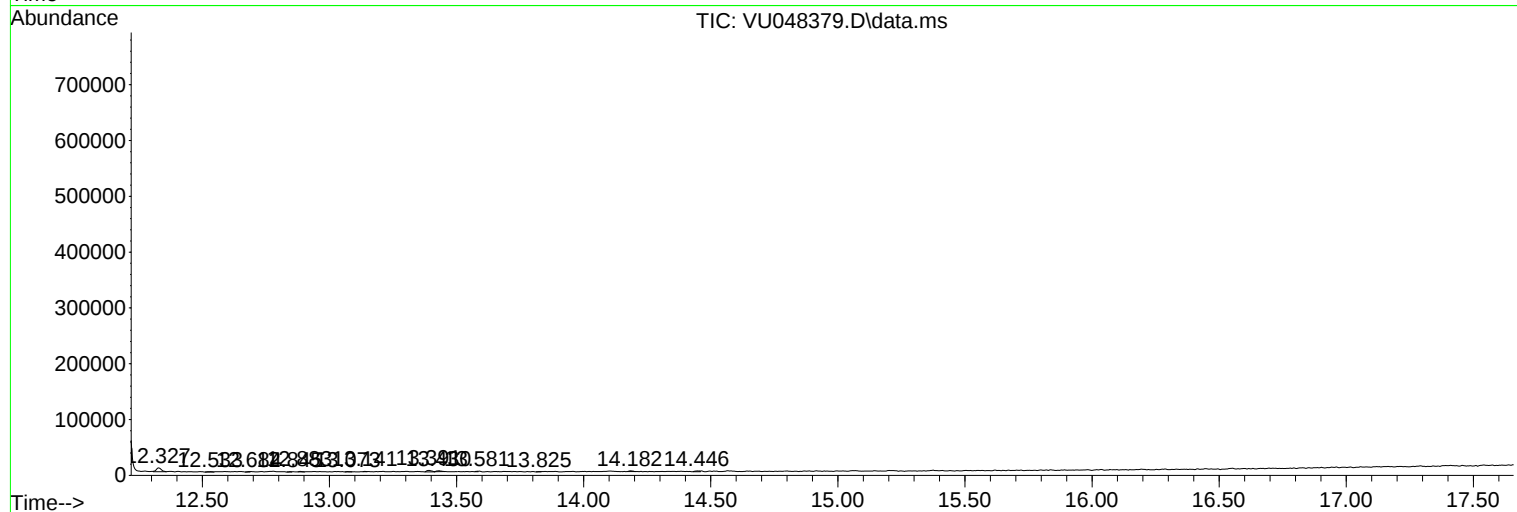
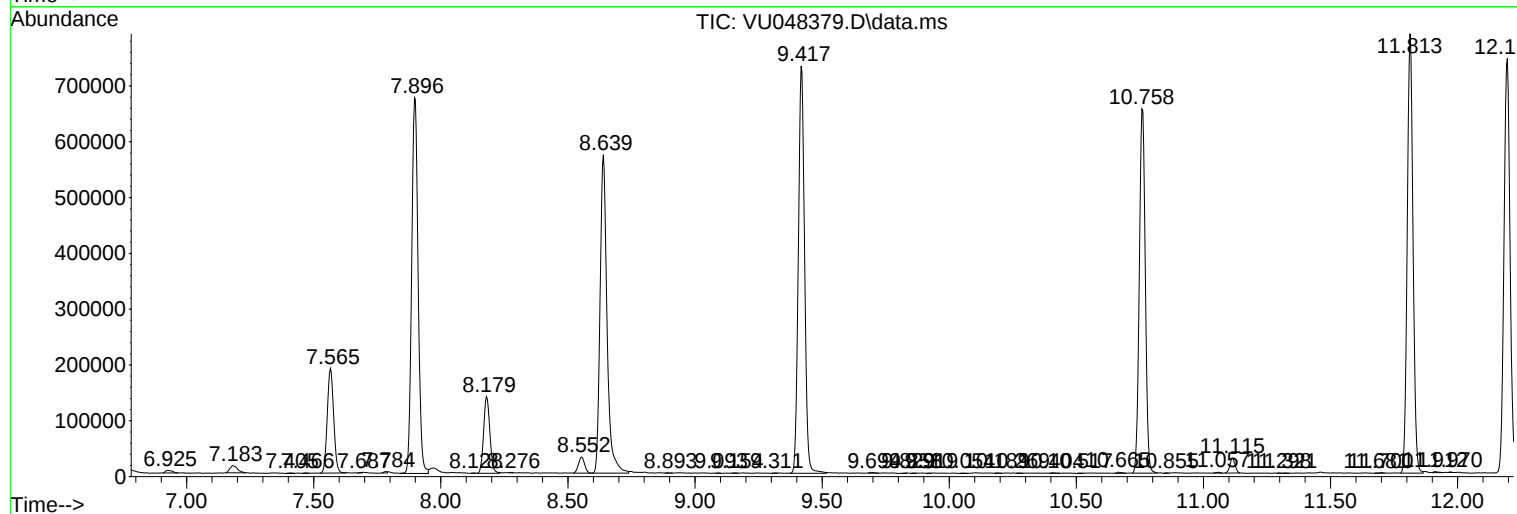
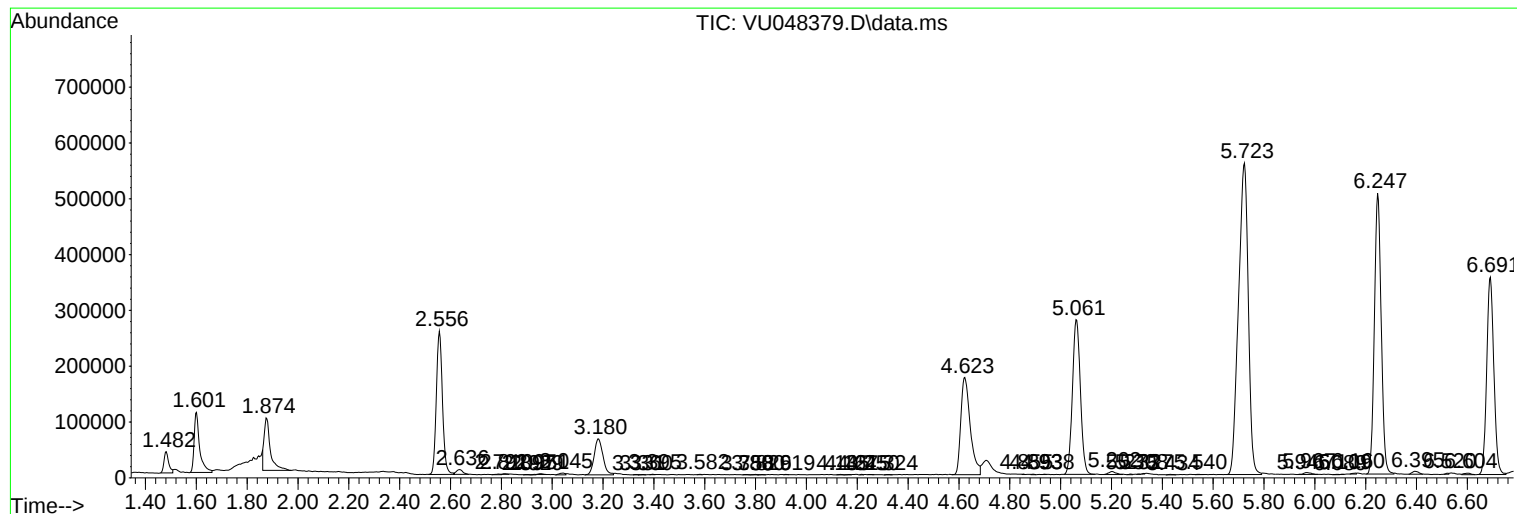
Sum of corrected areas: 12933412

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ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
EXL04ME

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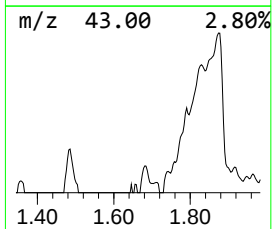
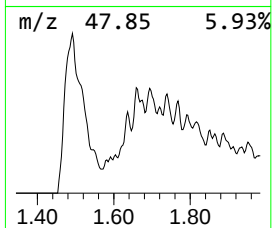
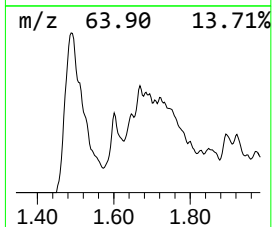
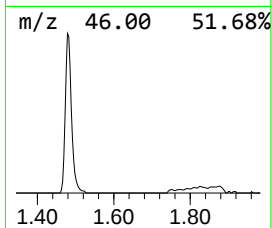
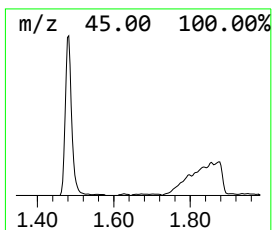
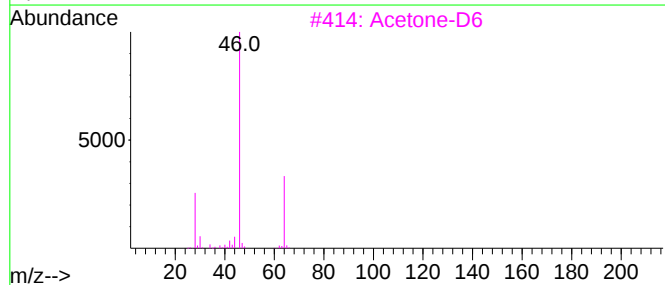
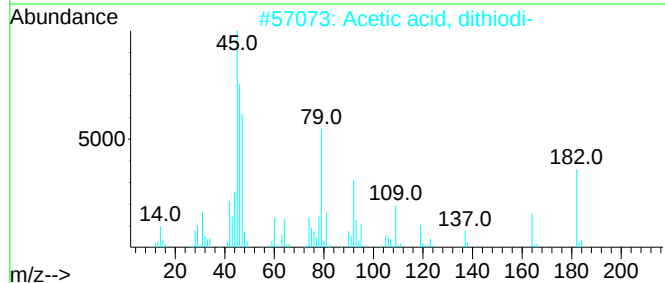
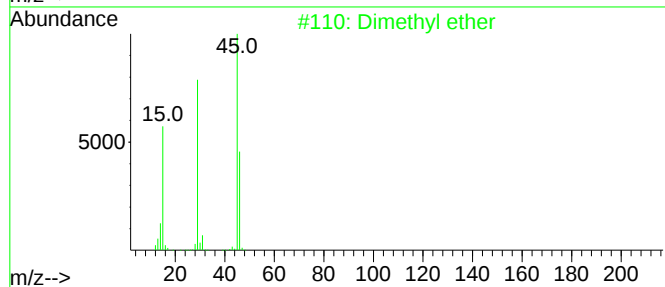
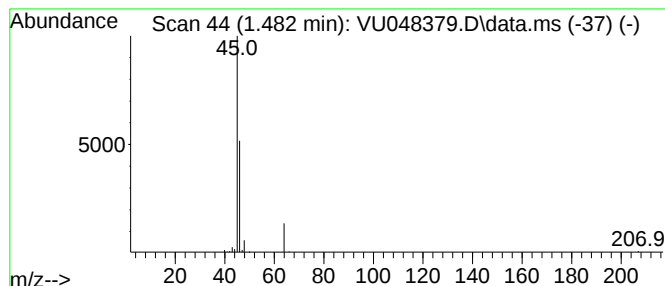
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Dimethyl ether Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.482	2.61 ug/L	49145	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl ether	46	C2H6O	000115-10-6	56
2			Acetic acid, dithiodi-	182	C4H6O4S2	000505-73-7	43
3			Acetone-D6	64	C3D6O	000666-52-4	9
4			Dimethyl ether	46	C2H6O	000115-10-6	9
5			Ethanol	46	C2H6O	000064-17-5	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Dimethyl ether	1.482	2.6	ug/L	49145	1	6.247	943176	50.0