

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV093024\
 Data File : VV037649.D
 Acq On : 30 Sep 2024 13:06
 Operator : SY/MD
 Sample : P4218-01 10X
 Misc : 5mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 E1H08

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092624WMA.M
 Title : VOC Analysis

Signal : TIC: VV037649.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.172	34	41	44	rBV3	7271	8931	0.33%	0.044%
2	1.278	67	74	93	rVB	373056	425243	15.68%	2.086%
3	1.416	109	117	118	rBV6	13830	13097	0.48%	0.064%
4	1.519	141	149	172	rVB	315778	404784	14.93%	1.986%
5	2.056	305	316	329	rBV	670121	981598	36.20%	4.816%
6	3.587	789	792	794	rVB3	853	490	0.02%	0.002%
7	3.606	794	798	801	rVB4	832	498	0.02%	0.002%
8	3.622	801	803	809	rBV2	563	442	0.02%	0.002%
9	3.664	813	816	822	rVB5	746	778	0.03%	0.004%
10	3.706	826	829	835	rVB5	935	898	0.03%	0.004%
11	3.735	835	838	842	rBV4	728	694	0.03%	0.003%
12	3.793	846	856	888	rBV	115270	324983	11.98%	1.594%
13	4.137	959	963	965	rBV4	818	687	0.03%	0.003%
14	4.149	965	967	970	rVB2	1396	705	0.03%	0.003%
15	4.243	974	996	1026	rBV	434304	1110661	40.96%	5.449%
16	4.394	1040	1043	1046	rVB4	810	503	0.02%	0.002%
17	4.474	1064	1068	1072	rBV4	1030	841	0.03%	0.004%
18	4.513	1075	1080	1084	rBV6	1352	1341	0.05%	0.007%
19	4.571	1092	1098	1101	rBV5	1428	1864	0.07%	0.009%
20	4.635	1114	1118	1123	rBV7	1116	1029	0.04%	0.005%
21	4.658	1123	1125	1129	rVV4	725	486	0.02%	0.002%
22	4.693	1129	1136	1139	rVB7	880	1050	0.04%	0.005%
23	4.728	1139	1147	1157	rVB10	1970	3348	0.12%	0.016%
24	4.789	1164	1166	1168	rBV3	955	502	0.02%	0.002%
25	4.821	1173	1176	1178	rVV4	990	550	0.02%	0.003%
26	4.834	1178	1180	1183	rVB4	855	466	0.02%	0.002%
27	4.947	1198	1215	1252	rBV3	1065044	2711813	100.00%	13.304%
28	5.220	1292	1300	1301	rBV7	3784	4284	0.16%	0.021%
29	5.352	1339	1341	1345	rVB4	967	644	0.02%	0.003%
30	5.455	1370	1373	1378	rVB6	1119	862	0.03%	0.004%
31	5.529	1385	1396	1426	rBV	735306	1526131	56.28%	7.487%
32	5.838	1478	1492	1495	rBV6	13477	28559	1.05%	0.140%
33	5.982	1525	1537	1568	rBV	595273	1245992	45.95%	6.113%
34	6.407	1663	1669	1701	rVB2	28945	72676	2.68%	0.357%
35	6.908	1815	1825	1855	rBV	332346	623168	22.98%	3.057%
36	7.120	1884	1891	1902	rBV3	20706	33713	1.24%	0.165%

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092624WMA.M
 Title : VOC Analysis

37	7.236	1916	1927	1945	rBV	1265665	2188597	80.71%	10.737%
38	7.548	2015	2024	2057	rBV	228057	437510	16.13%	2.146%
39	7.860	2112	2121	2134	rBV2	36829	66527	2.45%	0.326%
40	7.982	2152	2159	2161	rBV6	4444	5463	0.20%	0.027%
41	8.024	2163	2172	2197	rVV	385993	732368	27.01%	3.593%
42	8.509	2319	2323	2327	rBV5	1199	1121	0.04%	0.005%
43	8.619	2347	2357	2376	rBV	87807	151628	5.59%	0.744%
44	8.780	2395	2407	2438	rBV	1178660	1964770	72.45%	9.639%
45	9.075	2491	2499	2521	rVB	30459	59432	2.19%	0.292%
46	9.181	2528	2532	2540	rVB9	1216	1662	0.06%	0.008%
47	9.217	2540	2543	2544	rBV2	1001	598	0.02%	0.003%
48	9.255	2552	2555	2558	rBV5	1038	721	0.03%	0.004%
49	9.326	2574	2577	2579	rBV3	1320	885	0.03%	0.004%
50	9.480	2617	2625	2638	rBV2	21979	44260	1.63%	0.217%
51	9.558	2647	2649	2655	rVB5	2794	2227	0.08%	0.011%
52	9.667	2680	2683	2692	rVB8	2076	2863	0.11%	0.014%
53	9.702	2692	2694	2700	rBV5	887	736	0.03%	0.004%
54	9.873	2734	2747	2756	rBV6	6398	11996	0.44%	0.059%
55	9.943	2766	2769	2771	rBV4	715	443	0.02%	0.002%
56	10.021	2790	2793	2794	rBV2	889	523	0.02%	0.003%
57	10.091	2812	2815	2817	rBV3	1106	661	0.02%	0.003%
58	10.146	2817	2832	2848	rBV	704242	1101179	40.61%	5.402%
59	10.387	2901	2907	2914	rVV3	6583	9204	0.34%	0.045%
60	10.480	2924	2936	2943	rBV2	9552	16640	0.61%	0.082%
61	10.577	2961	2966	2970	rBV7	895	919	0.03%	0.005%
62	10.603	2970	2974	2978	rVB5	757	697	0.03%	0.003%
63	10.635	2982	2984	2989	rBV5	762	586	0.02%	0.003%
64	10.673	2989	2996	3007	rBV3	5681	8955	0.33%	0.044%
65	10.754	3018	3021	3025	rBV4	894	676	0.02%	0.003%
66	10.796	3025	3034	3042	rVV10	3239	5861	0.22%	0.029%
67	10.853	3044	3052	3065	rVV2	21610	36364	1.34%	0.178%
68	11.082	3121	3123	3127	rVB	717	451	0.02%	0.002%
69	11.127	3130	3137	3142	rBV6	5785	8345	0.31%	0.041%
70	11.178	3142	3153	3176	rBV	1182737	1875617	69.16%	9.202%
71	11.461	3234	3241	3247	rBV3	6622	9176	0.34%	0.045%
72	11.554	3258	3270	3295	rBV	1255486	2013404	74.25%	9.878%
73	11.744	3326	3329	3332	rBV5	1355	1092	0.04%	0.005%
74	11.953	3387	3394	3398	rBV7	2556	3632	0.13%	0.018%
75	12.046	3417	3423	3431	rBV7	1897	3439	0.13%	0.017%
76	12.239	3480	3483	3487	rBV	1291	1123	0.04%	0.006%

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 Title : VOC Analysis

77	12.406	3528	3535	3543	rVB7	4016	5299	0.20%	0.026%
78	12.586	3581	3591	3592	rBV5	4122	4439	0.16%	0.022%
79	12.696	3621	3625	3626	rBV3	812	528	0.02%	0.003%
80	12.773	3645	3649	3651	rBV5	852	736	0.03%	0.004%
81	12.818	3657	3663	3676	rVB9	7019	11839	0.44%	0.058%
82	12.930	3696	3698	3701	rBV3	596	430	0.02%	0.002%
83	12.950	3701	3704	3708	rVV4	906	878	0.03%	0.004%
84	13.001	3718	3720	3723	rVV2	1068	472	0.02%	0.002%
85	13.066	3738	3740	3744	rVB3	1132	749	0.03%	0.004%
86	13.101	3749	3751	3754	rVB2	753	450	0.02%	0.002%
87	13.207	3776	3784	3798	rBV2	5649	11081	0.41%	0.054%
88	13.313	3812	3817	3819	rBV4	866	678	0.03%	0.003%
89	13.332	3819	3823	3825	rBV3	1014	834	0.03%	0.004%
90	13.445	3846	3858	3869	rBV2	12384	25031	0.92%	0.123%
91	13.641	3916	3919	3924	rBV5	880	932	0.03%	0.005%
92	13.683	3924	3932	3939	rVV8	3899	6391	0.24%	0.031%
93	13.766	3952	3958	3960	rBV5	855	939	0.03%	0.005%
94	13.869	3987	3990	3992	rBV3	812	548	0.02%	0.003%
95	13.972	4019	4022	4023	rBV	1825	978	0.04%	0.005%
96	14.030	4037	4040	4043	rBV3	819	629	0.02%	0.003%
97	14.339	4133	4136	4138	rBV2	1197	727	0.03%	0.004%
98	14.397	4151	4154	4155	rBV3	872	592	0.02%	0.003%
99	14.680	4240	4242	4245	rBV2	1127	639	0.02%	0.003%
100	15.191	4398	4401	4403	rBV4	1281	970	0.04%	0.005%

Sum of corrected areas: 20383451

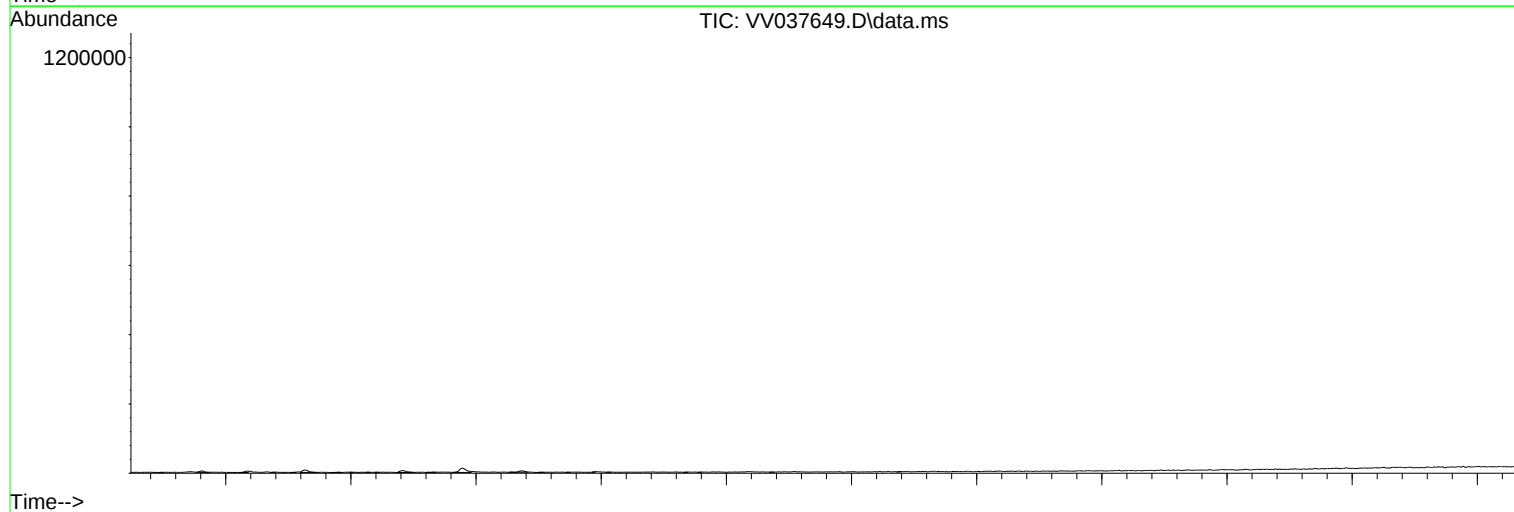
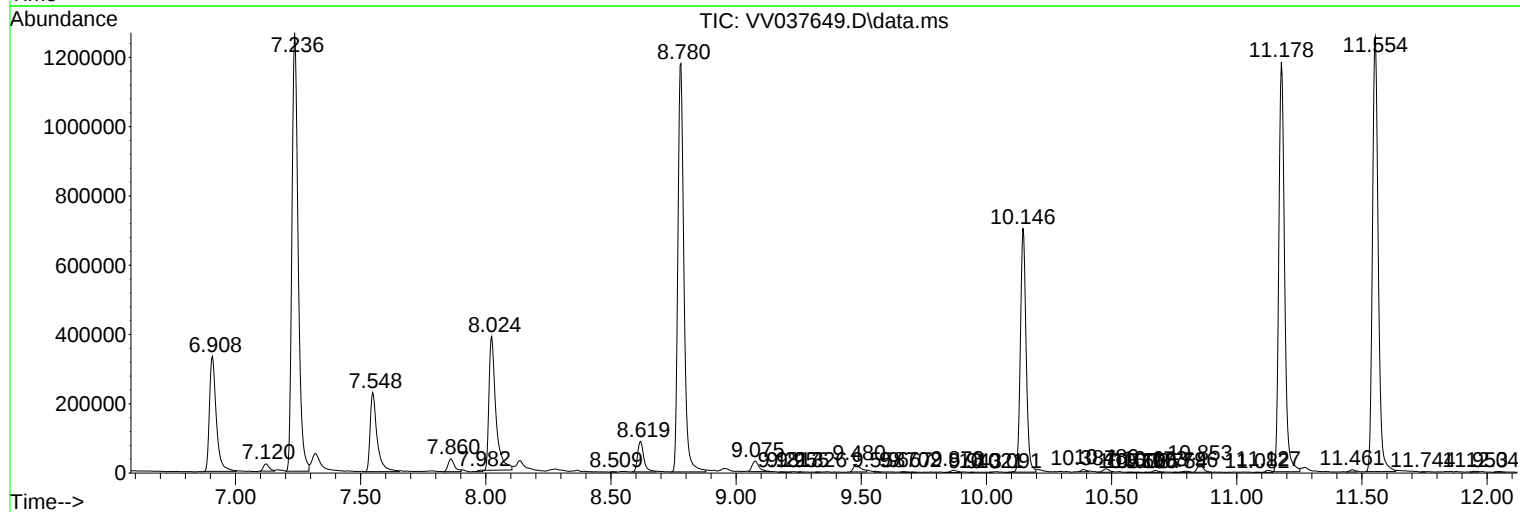
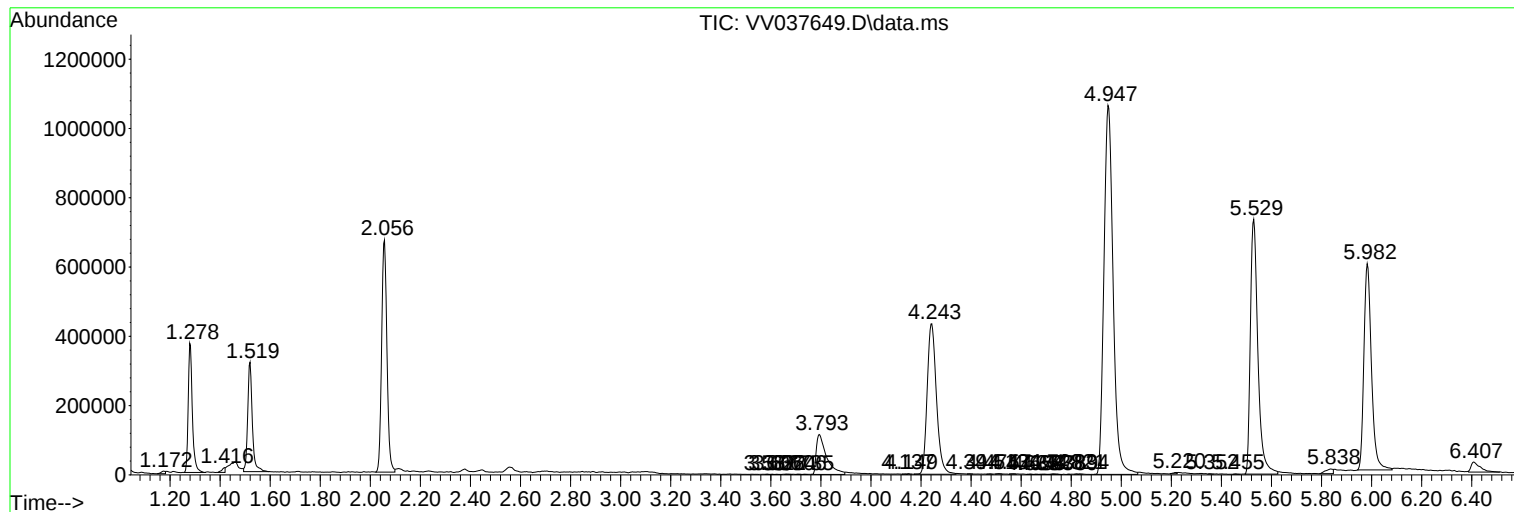
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ALS Vial : 1 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092624WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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Quant Title : VOC Analysis

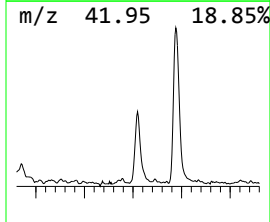
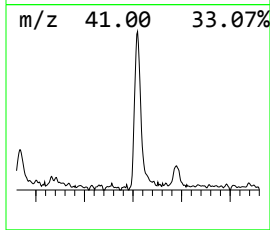
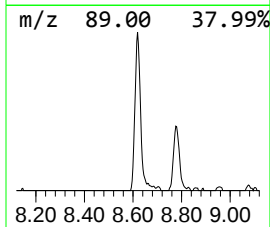
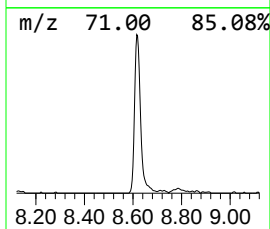
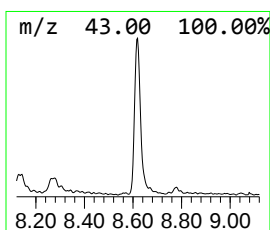
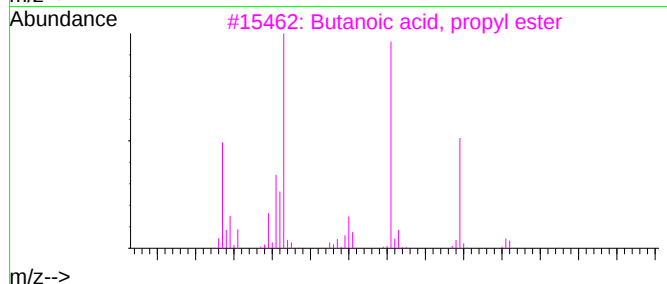
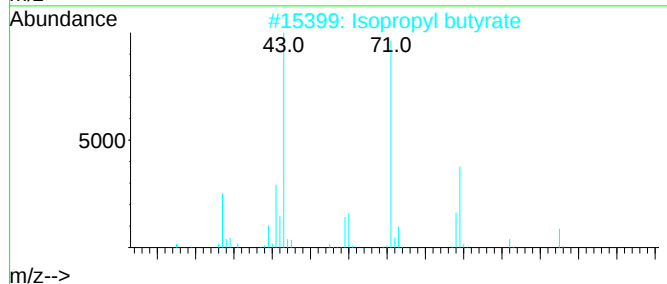
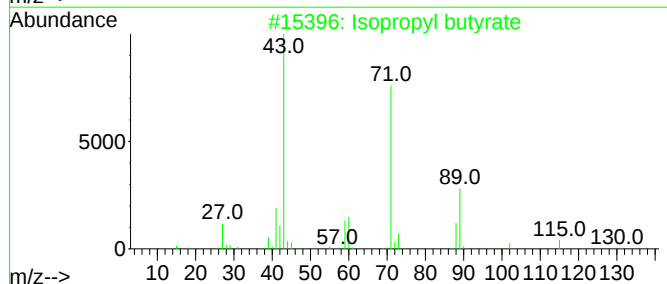
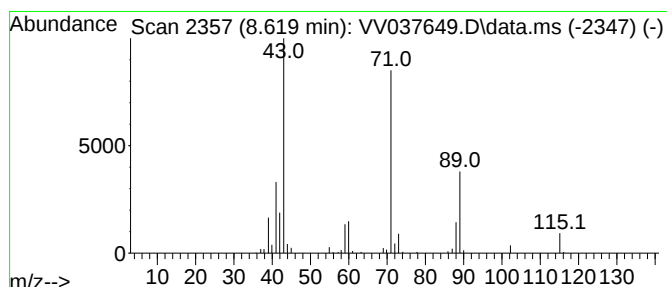
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 2 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.619	3.86 ug/L	151628	Chlorobenzene-d5	8.780

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	90
2	Isopropyl butyrate	130	C7H14O2	000638-11-9	90
3	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
4	Isopropyl butyrate	130	C7H14O2	000638-11-9	72
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72



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Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Isopropyl butyrate	8.619	3.9	ug/L	151628	2	8.780	1964770	50.0