

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072424\
 Data File : VX042487.D
 Acq On : 23 Jul 2024 21:09
 Operator : JC/MD
 Sample : P3327-18
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E20D8

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_X\Method\SFAMXML070324WMA.M
 Title : VOC Analysis

Signal : TIC: VX042487.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	22	25	32	rBV2	18809	25557	3.84%	0.488%
2	1.368	43	46	57	rVB	63201	78933	11.86%	1.508%
3	1.648	88	92	101	rVB	51528	67580	10.15%	1.291%
4	2.294	192	198	209	rBV	133528	215955	32.45%	4.126%
5	2.392	210	214	220	rVB	2108	3297	0.50%	0.063%
6	2.483	228	229	230	rBB	104	38	0.01%	0.001%
7	2.502	230	232	238	rBV3	219	396	0.06%	0.008%
8	2.605	248	249	252	rVB	188	119	0.02%	0.002%
9	2.788	274	279	284	rBV3	892	1483	0.22%	0.028%
10	2.886	293	295	296	rBV	130	71	0.01%	0.001%
11	2.947	299	305	310	rBV2	696	1553	0.23%	0.030%
12	3.056	321	323	325	rVB	153	104	0.02%	0.002%
13	3.087	325	328	333	rBV3	248	447	0.07%	0.009%
14	3.154	337	339	340	rBV	111	55	0.01%	0.001%
15	3.197	345	346	347	rBV	82	40	0.01%	0.001%
16	3.306	362	364	366	rBV2	261	227	0.03%	0.004%
17	3.337	366	369	372	rBV2	143	264	0.04%	0.005%
18	3.416	378	382	383	rBV2	126	129	0.02%	0.002%
19	3.459	388	389	394	rBV2	133	222	0.03%	0.004%
20	3.550	402	404	406	rBV2	186	207	0.03%	0.004%
21	3.660	419	422	424	rBV2	152	240	0.04%	0.005%
22	3.763	438	439	442	rBV2	129	161	0.02%	0.003%
23	3.824	448	449	450	rBV	119	51	0.01%	0.001%
24	3.867	454	456	458	rBV2	71	72	0.01%	0.001%
25	4.001	477	478	479	rBV	152	81	0.01%	0.002%
26	4.038	482	484	485	rBV2	253	215	0.03%	0.004%
27	4.148	500	502	504	rBV2	141	167	0.03%	0.003%
28	4.385	538	541	542	rVB2	164	152	0.02%	0.003%
29	4.471	546	555	579	rBV2	51393	168646	25.34%	3.222%
30	4.867	618	620	621	rBV	155	103	0.02%	0.002%
31	4.952	633	634	635	rBV	110	52	0.01%	0.001%
32	5.056	640	651	666	rVV	84331	262488	39.44%	5.015%
33	5.306	691	692	695	rBV	146	105	0.02%	0.002%
34	5.336	695	697	699	rVB	136	93	0.01%	0.002%
35	5.373	702	703	705	rVB	166	66	0.01%	0.001%
36	5.391	705	706	712	rBV	318	293	0.04%	0.006%

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37	5.452	714	716	719	rBV2	160	176	0.03%	0.003%
38	5.495	721	723	725	rVB2	149	94	0.01%	0.002%
39	5.769	766	768	769	rBV	84	53	0.01%	0.001%
40	5.970	790	801	820	rBV2	228279	665560	100.00%	12.715%
41	6.306	854	856	858	rBV	165	141	0.02%	0.003%
42	6.342	861	862	865	rBV3	151	177	0.03%	0.003%
43	6.440	876	878	879	rBV	122	86	0.01%	0.002%
44	6.763	921	931	948	rBV	177077	428803	64.43%	8.192%
45	7.123	983	990	1003	rBV	69598	159176	23.92%	3.041%
46	7.306	1013	1020	1035	rBV	132621	296232	44.51%	5.659%
47	7.671	1078	1080	1081	rBV	118	48	0.01%	0.001%
48	7.781	1096	1098	1099	rBV	108	88	0.01%	0.002%
49	7.964	1124	1128	1132	rVV3	345	520	0.08%	0.010%
50	8.025	1136	1138	1141	rVB2	159	158	0.02%	0.003%
51	8.068	1141	1145	1147	rBV2	105	173	0.03%	0.003%
52	8.141	1155	1157	1161	rBV	102	123	0.02%	0.002%
53	8.171	1161	1162	1164	rBV	140	79	0.01%	0.002%
54	8.324	1181	1187	1199	rBV	74162	128982	19.38%	2.464%
55	8.519	1214	1219	1223	rBV4	465	852	0.13%	0.016%
56	8.580	1226	1229	1230	rBV2	237	231	0.03%	0.004%
57	8.647	1234	1240	1256	rBV	334734	539768	81.10%	10.312%
58	8.952	1285	1290	1308	rBV	53380	82589	12.41%	1.578%
59	9.281	1339	1344	1349	rVB2	4223	6446	0.97%	0.123%
60	9.317	1349	1350	1352	rBV	118	75	0.01%	0.001%
61	9.384	1356	1361	1380	rBV	204689	314395	47.24%	6.006%
62	9.537	1382	1386	1392	rVB2	2596	4705	0.71%	0.090%
63	9.695	1411	1412	1414	rBV2	194	156	0.02%	0.003%
64	9.848	1435	1437	1440	rVB2	210	145	0.02%	0.003%
65	9.878	1440	1442	1444	rBV	88	60	0.01%	0.001%
66	10.055	1465	1471	1484	rBV	363905	489385	73.53%	9.349%
67	10.311	1510	1513	1519	rVB	640	843	0.13%	0.016%
68	10.543	1549	1551	1553	rBV2	102	67	0.01%	0.001%
69	10.598	1559	1560	1561	rBV	95	46	0.01%	0.001%
70	10.652	1565	1569	1570	rBV2	388	470	0.07%	0.009%
71	10.793	1589	1592	1597	rVB2	257	382	0.06%	0.007%
72	10.963	1617	1620	1624	rBV	256	317	0.05%	0.006%
73	10.994	1624	1625	1627	rBV2	92	82	0.01%	0.002%
74	11.073	1636	1638	1640	rVB2	103	68	0.01%	0.001%
75	11.195	1652	1658	1670	rBV	251110	339974	51.08%	6.495%
76	11.311	1673	1677	1682	rVB	1621	2068	0.31%	0.040%

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 Title : VOC Analysis

77	11.354	1682	1684	1686	rBV2	80	63	0.01%	0.001%
78	11.451	1698	1700	1704	rVB2	171	163	0.02%	0.003%
79	11.762	1748	1751	1753	rBV	226	218	0.03%	0.004%
80	12.018	1788	1793	1806	rBV	336264	438236	65.84%	8.372%
81	12.219	1821	1826	1837	rBV	17343	26038	3.91%	0.497%
82	12.317	1837	1842	1852	rBV	369520	469903	70.60%	8.977%
83	12.609	1888	1890	1891	rBV	159	146	0.02%	0.003%
84	12.762	1912	1915	1918	rVB4	390	491	0.07%	0.009%
85	12.792	1918	1920	1921	rBV2	124	83	0.01%	0.002%
86	12.859	1928	1931	1935	rBV3	475	586	0.09%	0.011%
87	12.957	1945	1947	1948	rBV	114	67	0.01%	0.001%
88	12.994	1951	1953	1955	rVB	134	76	0.01%	0.001%
89	13.506	2035	2037	2040	rBV	216	206	0.03%	0.004%
90	13.695	2066	2068	2070	rVB	332	252	0.04%	0.005%
91	14.091	2132	2133	2135	rVB	202	75	0.01%	0.001%
92	14.121	2135	2138	2144	rBV2	720	1172	0.18%	0.022%
93	14.280	2162	2164	2166	rBV2	184	170	0.03%	0.003%
94	15.389	2342	2346	2350	rBV2	1881	2809	0.42%	0.054%
95	16.261	2487	2489	2490	rBV	485	295	0.04%	0.006%

Sum of corrected areas: 5234504

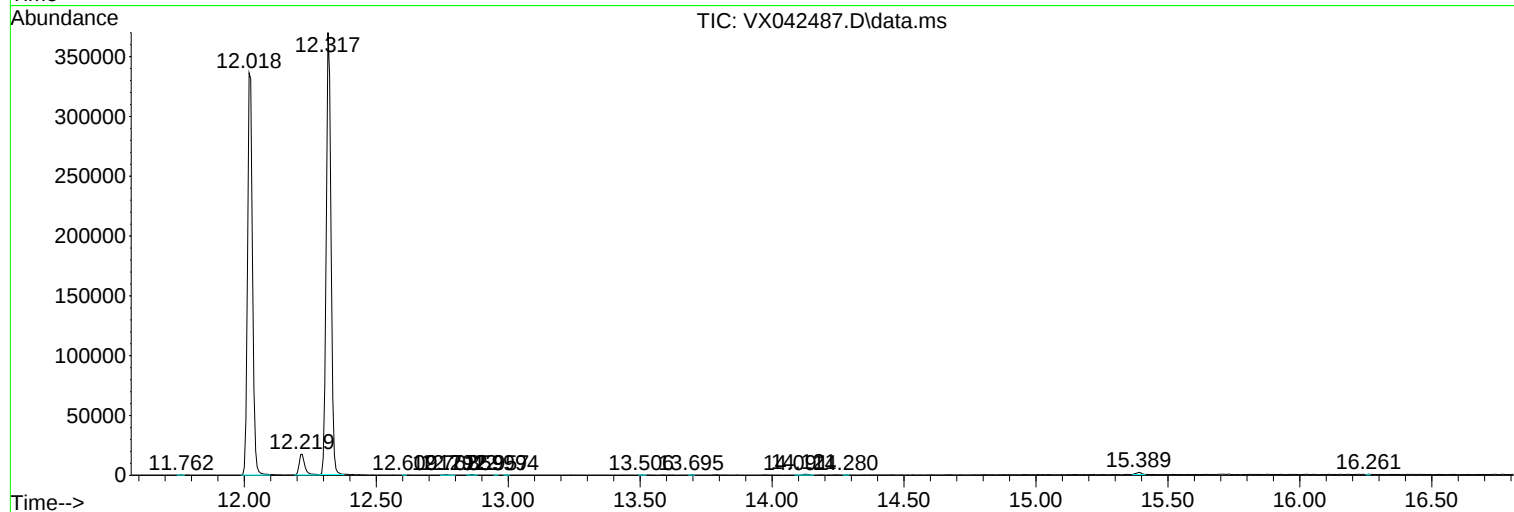
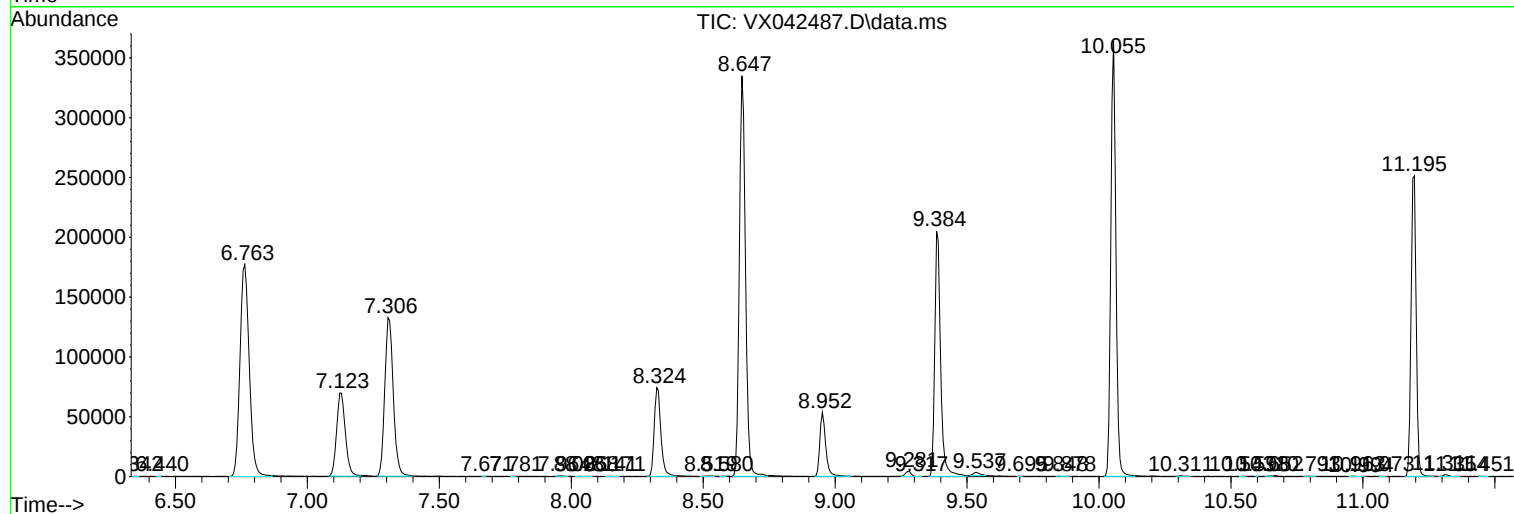
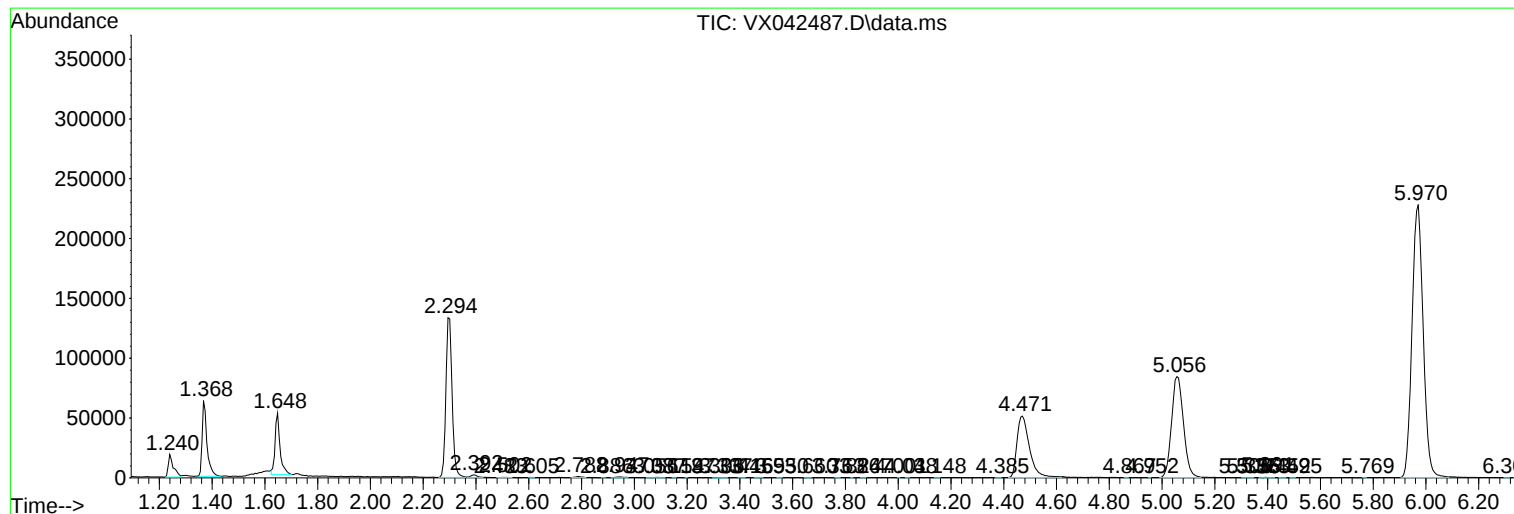
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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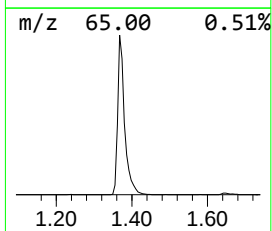
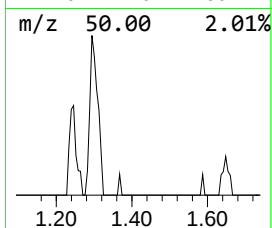
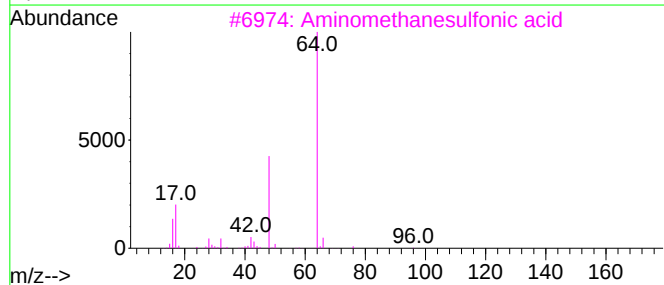
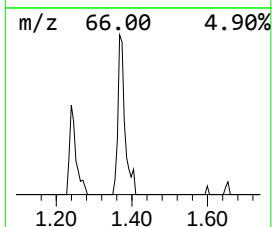
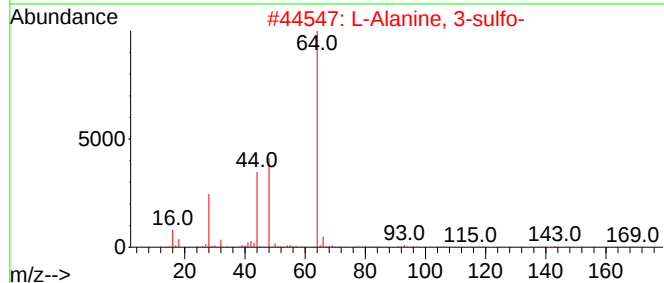
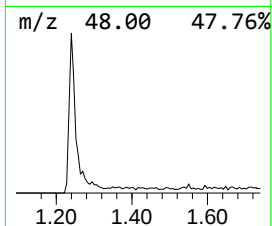
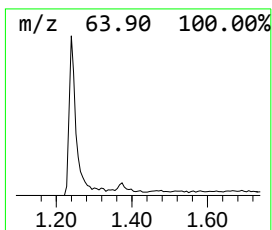
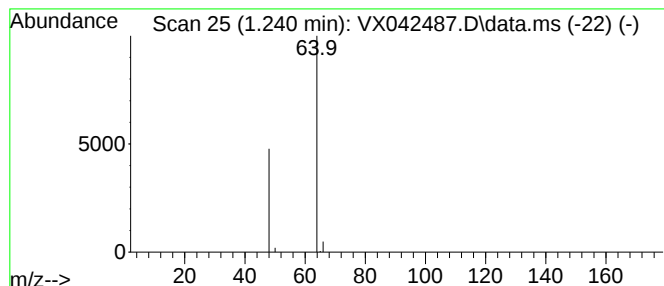
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	2.98 ug/L	25557	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
2			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			Sulfur dioxide	64	O2S	007446-09-5	4
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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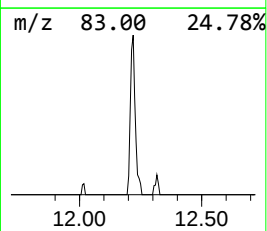
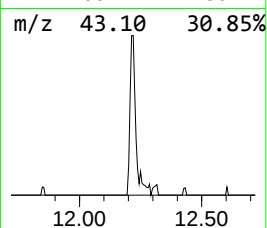
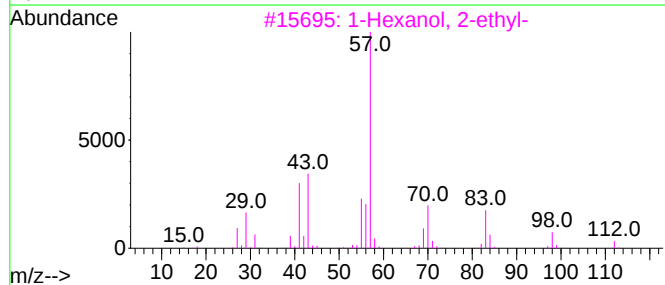
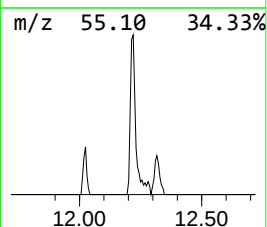
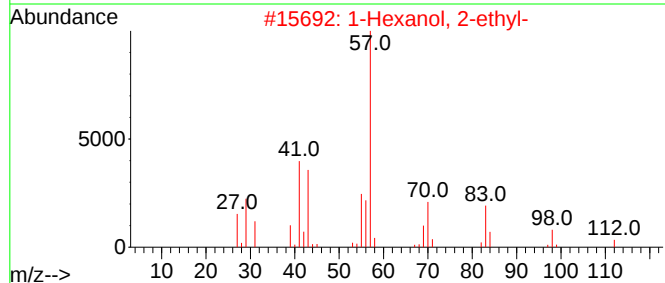
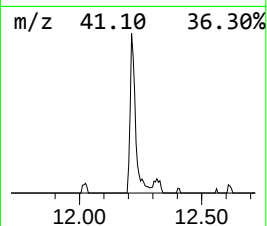
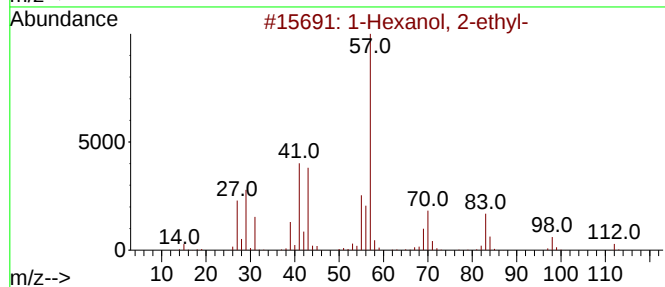
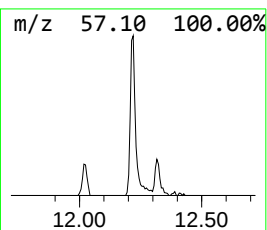
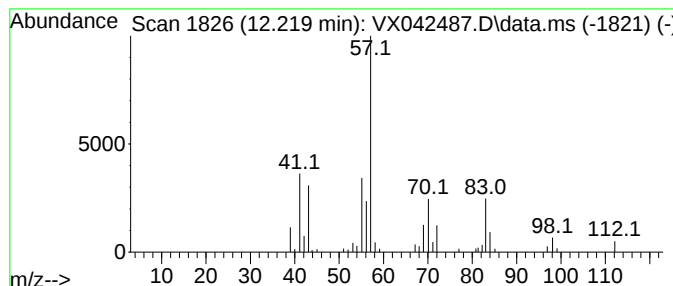
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	2.97 ug/L	26038	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
4			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	53
5			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	53



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.240	3.0	ug/L	25557	1	6.763	428803	50.0
1-Hexanol, 2-et...	12.219	3.0	ug/L	26038	3	12.024	438236	50.0