

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081822\
 Data File : VX030690.D
 Acq On : 18 Aug 2022 17:11
 Operator : JC/MD
 Sample : N4231-09
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0KQ6

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\SFAMXML080422WMA.M
 Title : VOC Analysis

Signal : TIC: VX030690.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	17	rVB	40483	36526	0.33%	0.112%
2	1.264	26	29	36	rBV3	12416	18110	0.16%	0.055%
3	1.368	42	46	54	rBV2	596180	666660	6.00%	2.043%
4	1.453	57	60	63	rVB	10643	9843	0.09%	0.030%
5	1.666	91	95	103	rVB	129179	157512	1.42%	0.483%
6	1.996	145	149	155	rVB	8918	12322	0.11%	0.038%
7	2.319	194	202	216	rBV	3175748	5149451	46.38%	15.779%
8	2.697	262	264	267	rVB2	790	749	0.01%	0.002%
9	2.727	267	269	273	rBV2	574	835	0.01%	0.003%
10	2.977	300	310	318	rVB5	1859	6025	0.05%	0.018%
11	3.093	323	329	338	rVV2	8860	17206	0.15%	0.053%
12	3.160	338	340	342	rVB2	408	405	0.00%	0.001%
13	3.276	356	359	363	rBV4	825	1299	0.01%	0.004%
14	3.337	367	369	372	rVB2	560	468	0.00%	0.001%
15	3.404	377	380	382	rBV	466	578	0.01%	0.002%
16	3.611	404	414	429	rVB2	127987	305159	2.75%	0.935%
17	3.727	432	433	436	rVB2	422	405	0.00%	0.001%
18	3.758	436	438	440	rBV2	449	413	0.00%	0.001%
19	3.873	454	457	458	rBV2	430	371	0.00%	0.001%
20	4.135	498	500	504	rBV3	344	517	0.00%	0.002%
21	4.166	504	505	506	rVB	645	236	0.00%	0.001%
22	4.178	506	507	508	rBV	501	290	0.00%	0.001%
23	4.221	512	514	515	rBV2	543	329	0.00%	0.001%
24	4.361	528	537	545	rBV3	7947	20406	0.18%	0.063%
25	4.495	546	559	584	rVV2	1291043	3698044	33.30%	11.332%
26	5.068	640	653	667	rBV2	171139	528783	4.76%	1.620%
27	5.208	674	676	677	rBV	446	270	0.00%	0.001%
28	5.385	697	705	716	rVB3	13717	42384	0.38%	0.130%
29	5.489	720	722	726	rVB2	412	432	0.00%	0.001%
30	5.550	727	732	734	rBV3	2271	3402	0.03%	0.010%
31	5.721	758	760	762	rBV	395	283	0.00%	0.001%
32	5.782	769	770	773	rVB2	495	401	0.00%	0.001%
33	5.977	790	802	817	rBV2	450788	1327724	11.96%	4.068%
34	6.342	858	862	863	rBV2	712	882	0.01%	0.003%
35	6.391	863	870	880	rVB2	8345	21419	0.19%	0.066%
36	6.580	899	901	902	rBV2	336	219	0.00%	0.001%

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 Title : VOC Analysis

37	6.769	919	932	948	rBV	307412	748293	6.74%	2.293%
38	7.037	974	976	979	rBV3	409	527	0.00%	0.002%
39	7.129	981	991	1013	rBV	5091116	11103580	100.00%	34.024%
40	7.312	1013	1021	1034	rVB	272752	597846	5.38%	1.832%
41	7.671	1074	1080	1093	rBV2	59114	126327	1.14%	0.387%
42	7.891	1114	1116	1117	rBV	841	617	0.01%	0.002%
43	8.208	1167	1168	1171	rBV2	299	275	0.00%	0.001%
44	8.330	1181	1188	1197	rBV	176708	290259	2.61%	0.889%
45	8.482	1210	1213	1215	rBV3	1056	1513	0.01%	0.005%
46	8.653	1234	1241	1249	rBV	702933	1070601	9.64%	3.281%
47	8.726	1249	1253	1256	rVB4	5043	7094	0.06%	0.022%
48	8.848	1270	1273	1281	rVB2	8287	14538	0.13%	0.045%
49	8.909	1281	1283	1284	rBV	382	327	0.00%	0.001%
50	8.952	1285	1290	1298	rBV	122950	188060	1.69%	0.576%
51	9.171	1320	1326	1333	rBV6	6632	12734	0.11%	0.039%
52	9.275	1333	1343	1354	rBV	1652367	2396933	21.59%	7.345%
53	9.385	1356	1361	1377	rVV	471125	687245	6.19%	2.106%
54	9.525	1382	1384	1387	rBV4	1839	1982	0.02%	0.006%
55	9.738	1414	1419	1423	rVB3	5797	7755	0.07%	0.024%
56	9.927	1448	1450	1453	rBV4	386	648	0.01%	0.002%
57	10.000	1458	1462	1465	rBV3	2298	4013	0.04%	0.012%
58	10.055	1466	1471	1481	rVB	647970	864520	7.79%	2.649%
59	10.250	1501	1503	1504	rBV2	574	326	0.00%	0.001%
60	10.275	1504	1507	1510	rBV4	1164	1516	0.01%	0.005%
61	10.378	1519	1524	1535	rBV	35073	48711	0.44%	0.149%
62	10.451	1535	1536	1540	rBV2	714	647	0.01%	0.002%
63	10.579	1555	1557	1560	rVB4	1189	1148	0.01%	0.004%
64	10.622	1560	1564	1566	rBV2	540	762	0.01%	0.002%
65	10.732	1580	1582	1583	rBV	744	432	0.00%	0.001%
66	10.848	1598	1601	1603	rBV2	597	669	0.01%	0.002%
67	11.012	1626	1628	1633	rVB4	1759	1977	0.02%	0.006%
68	11.195	1652	1658	1666	rVB	488662	628455	5.66%	1.926%
69	11.311	1674	1677	1681	rVB4	983	1575	0.01%	0.005%
70	11.427	1691	1696	1699	rBV3	1499	2361	0.02%	0.007%
71	11.634	1728	1730	1732	rVB2	407	268	0.00%	0.001%
72	11.756	1748	1750	1751	rBV2	407	300	0.00%	0.001%
73	11.866	1766	1768	1769	rBV	442	260	0.00%	0.001%
74	11.933	1776	1779	1782	rVB3	1300	1597	0.01%	0.005%
75	12.024	1789	1794	1803	rBV	688485	829114	7.47%	2.541%
76	12.232	1823	1828	1830	rBV4	3014	5069	0.05%	0.016%

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77	12.323	1837	1843	1853	rBV	739393	912967	8.22%	2.798%
78	12.530	1875	1877	1879	rBV	590	438	0.00%	0.001%
79	12.555	1879	1881	1883	rVB3	749	556	0.01%	0.002%
80	12.597	1886	1888	1890	rBV2	733	728	0.01%	0.002%
81	12.768	1912	1916	1919	rBV3	1291	2075	0.02%	0.006%
82	12.811	1919	1923	1927	rVV3	3236	4653	0.04%	0.014%
83	12.860	1927	1931	1937	rVB4	2146	3440	0.03%	0.011%
84	12.951	1944	1946	1950	rBV2	716	985	0.01%	0.003%
85	13.061	1962	1964	1966	rBV2	552	489	0.00%	0.001%
86	13.158	1978	1980	1982	rBV2	591	501	0.00%	0.002%
87	13.481	2032	2033	2037	rVB2	577	485	0.00%	0.001%
88	13.585	2048	2050	2054	rBV4	907	919	0.01%	0.003%
89	13.689	2065	2067	2071	rVB2	1105	1204	0.01%	0.004%
90	14.000	2116	2118	2122	rBV3	539	621	0.01%	0.002%
91	14.134	2137	2140	2143	rVB3	1535	2004	0.02%	0.006%
92	14.213	2150	2153	2155	rBV2	725	698	0.01%	0.002%
93	14.262	2159	2161	2163	rBV2	692	789	0.01%	0.002%
94	14.384	2179	2181	2182	rVB	842	504	0.00%	0.002%
95	14.725	2235	2237	2240	rBV2	1140	859	0.01%	0.003%
96	14.945	2271	2273	2275	rBV2	898	600	0.01%	0.002%
97	15.182	2309	2312	2314	rBV3	993	1159	0.01%	0.004%
98	15.383	2341	2345	2346	rBV3	1318	1620	0.01%	0.005%
99	15.493	2358	2363	2369	rVB	10859	14310	0.13%	0.044%
100	16.572	2538	2540	2543	rBV2	1006	902	0.01%	0.003%

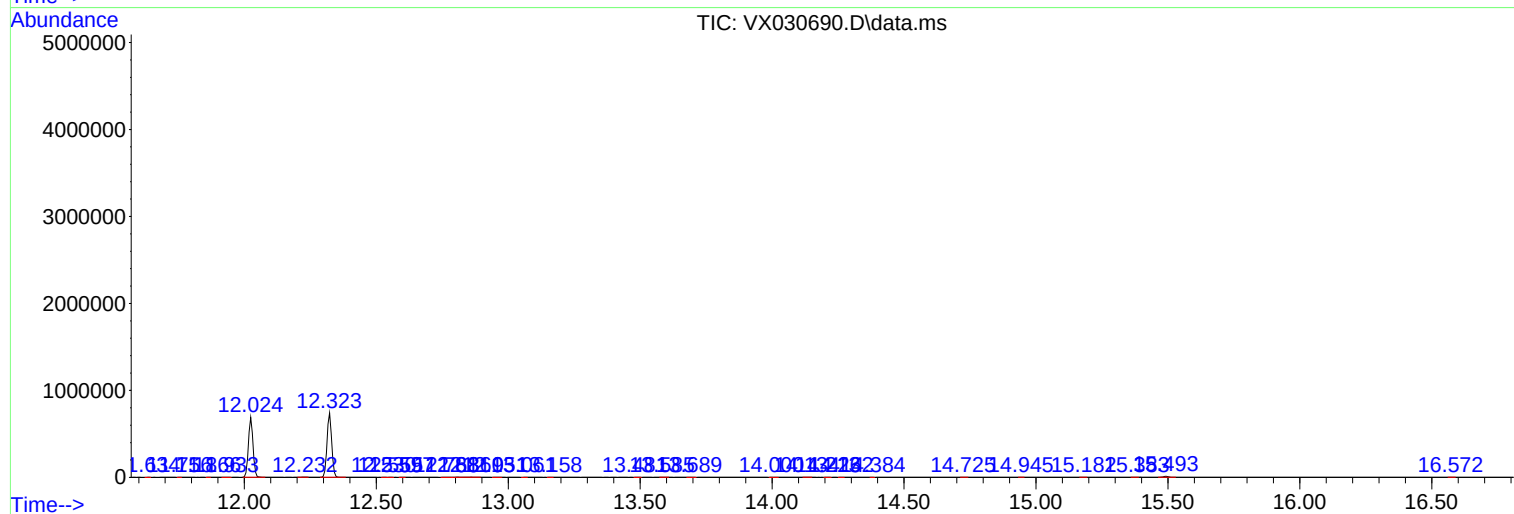
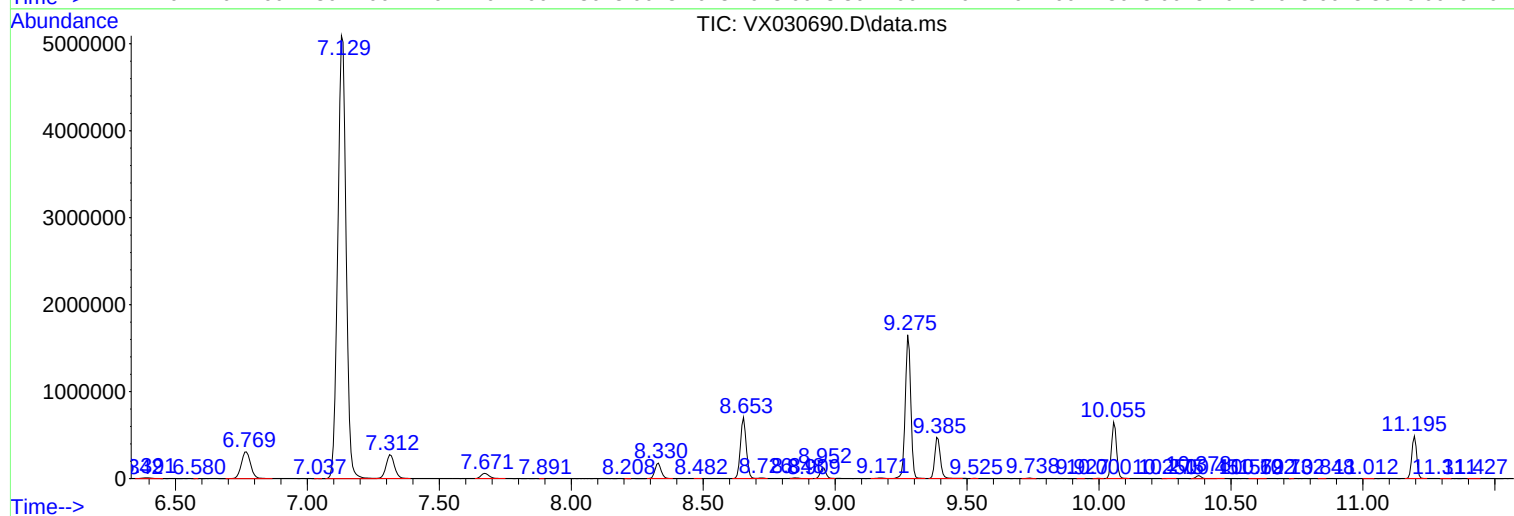
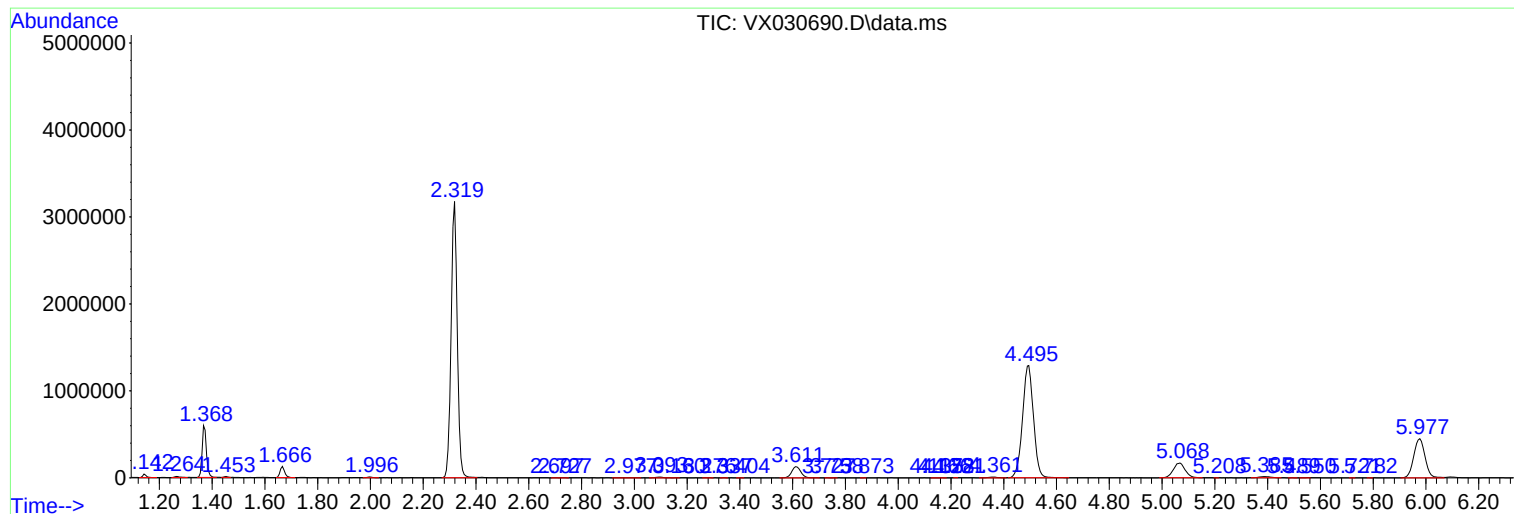
Sum of corrected areas: 32634738

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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



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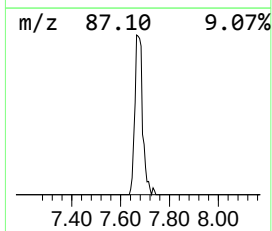
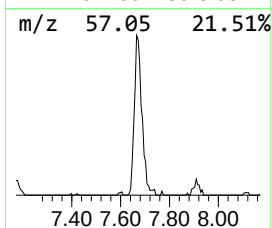
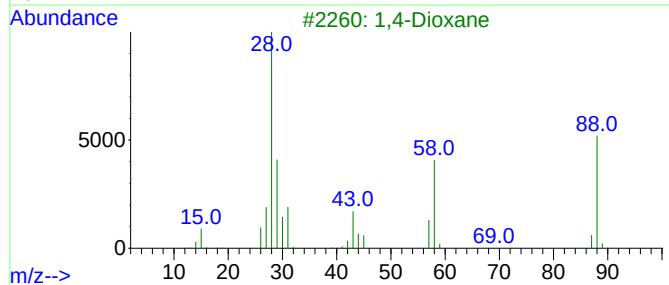
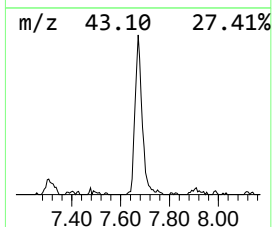
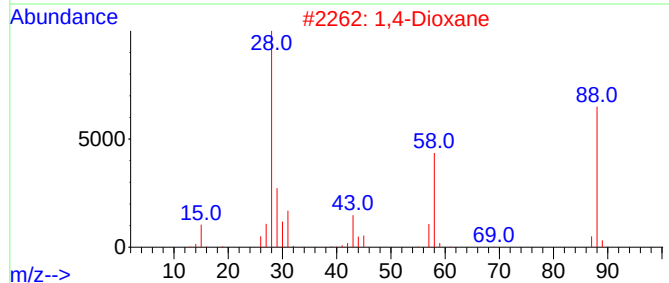
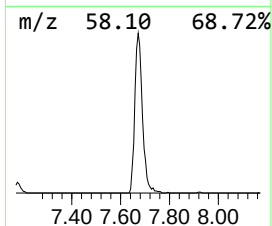
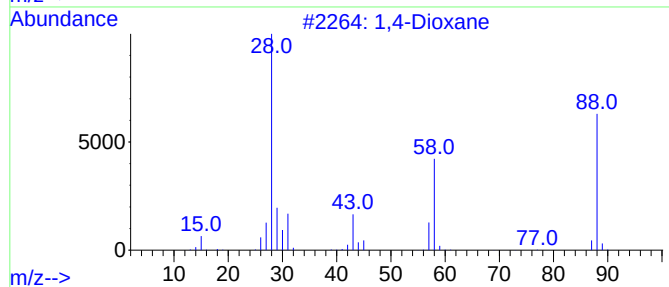
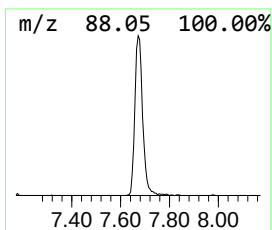
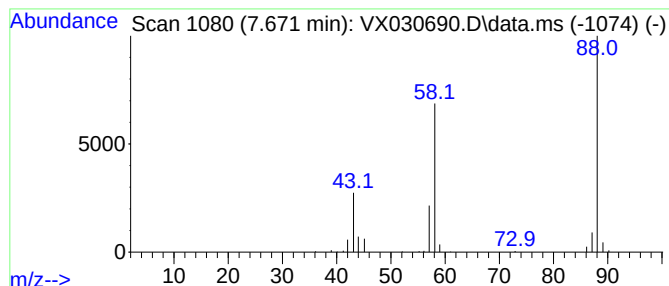
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 1,4-Dioxane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.671	8.44 ug/L	126327	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dioxane			88	C4H8O2	000123-91-1	91
2	1,4-Dioxane			88	C4H8O2	000123-91-1	86
3	1,4-Dioxane			88	C4H8O2	000123-91-1	83
4	1,4-Dioxane			88	C4H8O2	000123-91-1	83
5	1,4-Dioxane			88	C4H8O2	000123-91-1	72



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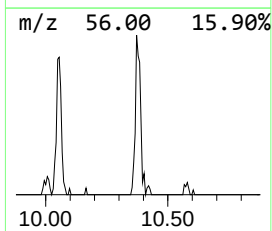
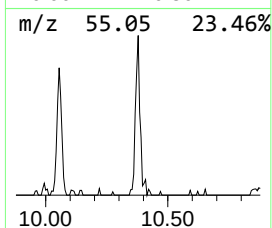
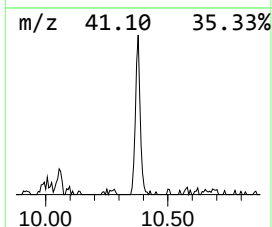
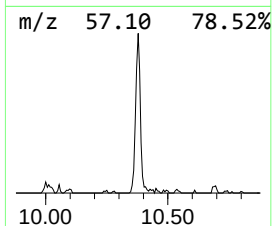
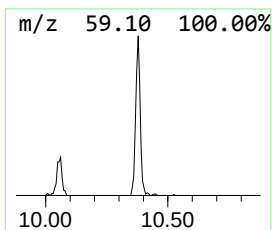
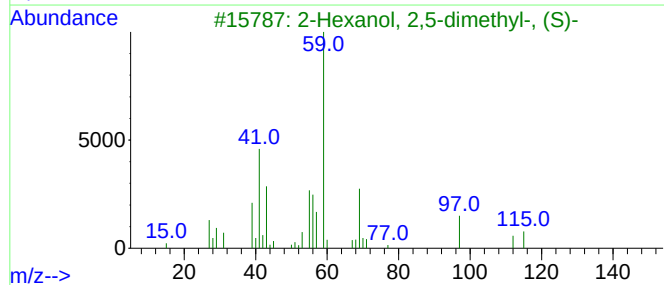
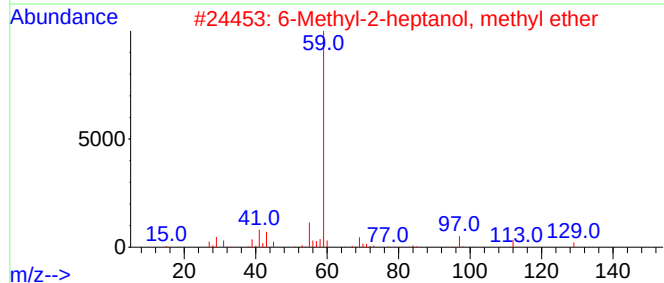
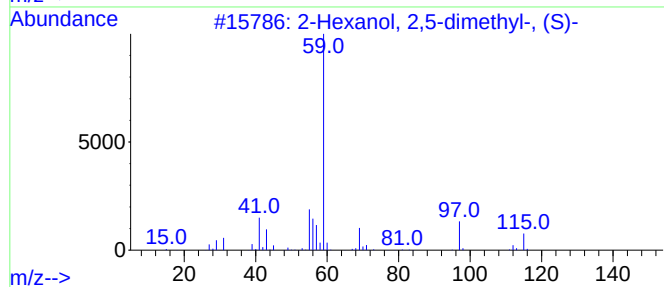
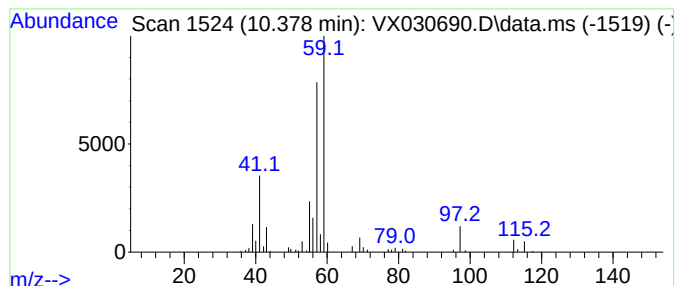
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.378	2.82 ug/L	48711	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	56
2			6-Methyl-2-heptanol, methyl ether	144	C9H20O	1000365-52-0	53
3			2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	38
4			Propane, 1-(1,1-dimethylethoxy)-...	130	C8H18O	033021-02-2	33
5			Ethanol, 2-(1,1-dimethylethoxy)-	118	C6H14O2	007580-85-0	33



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,4-Dioxane	7.671	8.4	ug/L	126327	1	6.769	748293	50.0
2-Hexanol, 2,5-...	10.378	2.8	ug/L	48711	2	10.055	864520	50.0