

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042623\
 Data File : VX035319.D
 Acq On : 26 Apr 2023 17:30
 Operator : JC/MD
 Sample : 02479-12ME
 Misc : 5.08g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EW953ME

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\SFAMXML041823WMA.M
 Title : VOC Analysis

Signal : TIC: VX035319.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	26	29	31	rBV	2702	2277	0.16%	0.018%
2	1.367	42	46	66	rVB	61735	139153	9.85%	1.112%
3	1.648	87	92	93	rBV	6778	9018	0.64%	0.072%
4	1.672	93	96	100	rBV	28547	40698	2.88%	0.325%
5	2.288	190	197	212	rBV	255337	417268	29.53%	3.334%
6	2.715	263	267	273	rVV2	1659	2782	0.20%	0.022%
7	2.782	273	278	288	rVV3	4080	9328	0.66%	0.075%
8	3.428	378	384	391	rVB4	1081	2630	0.19%	0.021%
9	4.482	548	557	584	rBV	78192	301161	21.31%	2.406%
10	5.056	639	651	668	rBV	172527	543024	38.43%	4.339%
11	5.306	687	692	700	rVV3	1109	3461	0.24%	0.028%
12	5.549	724	732	741	rVB6	1958	5711	0.40%	0.046%
13	5.964	788	800	815	rBV2	498672	1412968	100.00%	11.290%
14	6.366	858	866	874	rBV6	2304	6840	0.48%	0.055%
15	6.756	921	930	947	rBV	413945	991565	70.18%	7.923%
16	7.013	967	972	980	rVB5	977	2458	0.17%	0.020%
17	7.116	982	989	998	rBV7	4274	12942	0.92%	0.103%
18	7.214	998	1005	1011	rBV2	4340	10097	0.71%	0.081%
19	7.305	1011	1020	1036	rVB	299027	654109	46.29%	5.227%
20	7.482	1044	1049	1055	rBV4	1041	2369	0.17%	0.019%
21	7.775	1091	1097	1103	rVB6	1589	3063	0.22%	0.024%
22	7.957	1120	1127	1137	rBV6	5824	15056	1.07%	0.120%
23	8.226	1167	1171	1174	rVV4	1617	2714	0.19%	0.022%
24	8.268	1174	1178	1181	rVV3	3419	5185	0.37%	0.041%
25	8.323	1181	1187	1202	rVV	164652	278402	19.70%	2.225%
26	8.439	1202	1206	1211	rVV6	2664	5658	0.40%	0.045%
27	8.506	1212	1217	1224	rVV7	2118	5285	0.37%	0.042%
28	8.646	1234	1240	1255	rVB	746671	1155820	81.80%	9.235%
29	8.909	1279	1283	1285	rBV2	4763	6114	0.43%	0.049%
30	8.951	1285	1290	1305	rVV	114625	190833	13.51%	1.525%
31	9.104	1311	1315	1320	rVV4	1415	2227	0.16%	0.018%
32	9.158	1320	1324	1329	rVV4	1820	2810	0.20%	0.022%
33	9.274	1337	1343	1350	rVB3	18955	32749	2.32%	0.262%
34	9.390	1356	1362	1364	rBV	138864	215301	15.24%	1.720%
35	9.421	1364	1367	1378	rVB	238015	416777	29.50%	3.330%
36	9.616	1393	1399	1404	rBV	34794	55008	3.89%	0.440%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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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\SFAMXML041823WMA.M
 Title : VOC Analysis

37	9.756	1415	1422	1427	rVB3	9012	16881	1.19%	0.135%
38	9.829	1428	1434	1438	rBV4	6831	16310	1.15%	0.130%
39	9.902	1442	1446	1451	rVB4	5302	8259	0.58%	0.066%
40	10.012	1456	1464	1466	rBV2	9120	16431	1.16%	0.131%
41	10.055	1466	1471	1487	rVB	800852	1113269	78.79%	8.895%
42	10.177	1487	1491	1499	rVB6	4436	8438	0.60%	0.067%
43	10.274	1503	1507	1510	rBV5	5253	9493	0.67%	0.076%
44	10.359	1517	1521	1526	rBV3	15286	20700	1.47%	0.165%
45	10.457	1532	1537	1543	rBV2	11528	17771	1.26%	0.142%
46	10.536	1546	1550	1551	rBV2	1810	1858	0.13%	0.015%
47	10.585	1551	1558	1566	rVB4	10172	21360	1.51%	0.171%
48	10.670	1566	1572	1575	rBV4	5901	11444	0.81%	0.091%
49	10.780	1582	1590	1594	rBV	30778	48625	3.44%	0.389%
50	10.896	1605	1609	1614	rVB	26325	37290	2.64%	0.298%
51	10.951	1614	1618	1622	rVB5	5739	9033	0.64%	0.072%
52	11.000	1623	1626	1628	rBV3	5033	5845	0.41%	0.047%
53	11.030	1628	1631	1634	rVB3	6428	7006	0.50%	0.056%
54	11.085	1634	1640	1643	rBV3	14135	20920	1.48%	0.167%
55	11.201	1650	1659	1670	rBV	447476	727680	51.50%	5.814%
56	11.329	1675	1680	1685	rBV4	9193	18680	1.32%	0.149%
57	11.432	1694	1697	1700	rBV3	9289	10863	0.77%	0.087%
58	11.475	1701	1704	1709	rVB	38686	50138	3.55%	0.401%
59	11.634	1727	1730	1734	rVB2	8391	9985	0.71%	0.080%
60	11.682	1734	1738	1740	rBV4	7820	9236	0.65%	0.074%
61	11.713	1740	1743	1747	rBV	56259	69541	4.92%	0.556%
62	11.841	1759	1764	1765	rBV5	6080	9060	0.64%	0.072%
63	11.890	1769	1772	1777	rVV5	18830	30117	2.13%	0.241%
64	11.945	1778	1781	1784	rVV4	9887	15068	1.07%	0.120%
65	11.975	1784	1786	1789	rVV4	9587	9814	0.69%	0.078%
66	12.024	1789	1794	1800	rVV	858706	1109278	78.51%	8.863%
67	12.073	1800	1802	1805	rVV3	11208	13896	0.98%	0.111%
68	12.103	1805	1807	1811	rVB5	10101	11197	0.79%	0.089%
69	12.158	1811	1816	1825	rVB5	18348	38909	2.75%	0.311%
70	12.243	1826	1830	1833	rBV6	4959	10251	0.73%	0.082%
71	12.323	1838	1843	1849	rBV	854892	1081426	76.54%	8.641%
72	12.426	1856	1860	1864	rBV	61475	70420	4.98%	0.563%
73	12.463	1864	1866	1873	rVB6	15930	28210	2.00%	0.225%
74	12.560	1876	1882	1883	rBV6	9454	18489	1.31%	0.148%
75	12.682	1898	1902	1905	rBV5	20218	25985	1.84%	0.208%
76	12.761	1913	1915	1920	rVB4	9857	11870	0.84%	0.095%

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Instrument :
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 ClientSampleId :
 EW953ME

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

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Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
 Title : VOC Analysis

77	12.816	1922	1924	1929	rVB5	11876	13279	0.94%	0.106%
78	12.890	1931	1936	1943	rVV7	26154	58540	4.14%	0.468%
79	12.944	1943	1945	1946	rVV	5658	4809	0.34%	0.038%
80	12.975	1948	1950	1955	rVB4	14560	20387	1.44%	0.163%
81	13.042	1958	1961	1964	rBV4	10671	11422	0.81%	0.091%
82	13.146	1974	1978	1981	rBV6	6460	10990	0.78%	0.088%
83	13.268	1994	1998	2001	rBV	93783	112953	7.99%	0.903%
84	13.383	2013	2017	2020	rBV	60639	76016	5.38%	0.607%
85	13.676	2063	2065	2067	rBV3	11148	14082	1.00%	0.113%
86	13.706	2067	2070	2072	rVB3	21606	25788	1.83%	0.206%
87	13.798	2082	2085	2088	rVB2	29261	33670	2.38%	0.269%
88	13.841	2089	2092	2096	rVB2	24529	30550	2.16%	0.244%
89	14.036	2121	2124	2128	rVB	76064	84100	5.95%	0.672%
90	14.103	2132	2135	2138	rBV4	16192	22096	1.56%	0.177%
91	14.133	2138	2140	2144	rVB3	14695	16606	1.18%	0.133%
92	14.615	2216	2219	2221	rBV	18637	22189	1.57%	0.177%
93	14.725	2234	2237	2238	rBV2	7634	8424	0.60%	0.067%
94	14.755	2239	2242	2245	rVB	41158	42799	3.03%	0.342%
95	14.883	2260	2263	2267	rVB	23409	28603	2.02%	0.229%
96	15.035	2286	2288	2292	rBV2	7677	11054	0.78%	0.088%
97	15.133	2300	2304	2308	rBV	32002	40454	2.86%	0.323%
98	15.487	2358	2362	2367	rBV3	18102	28763	2.04%	0.230%
99	15.645	2384	2388	2397	rVB2	31800	56523	4.00%	0.452%
100	16.273	2487	2491	2492	rBV4	5445	7190	0.51%	0.057%

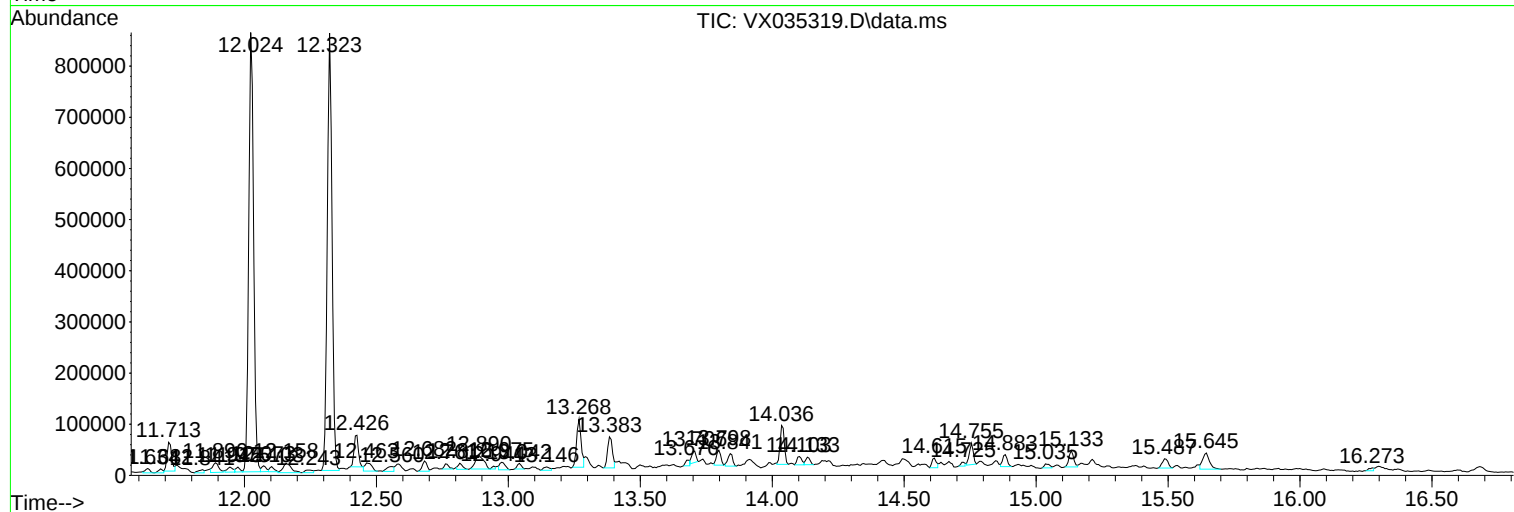
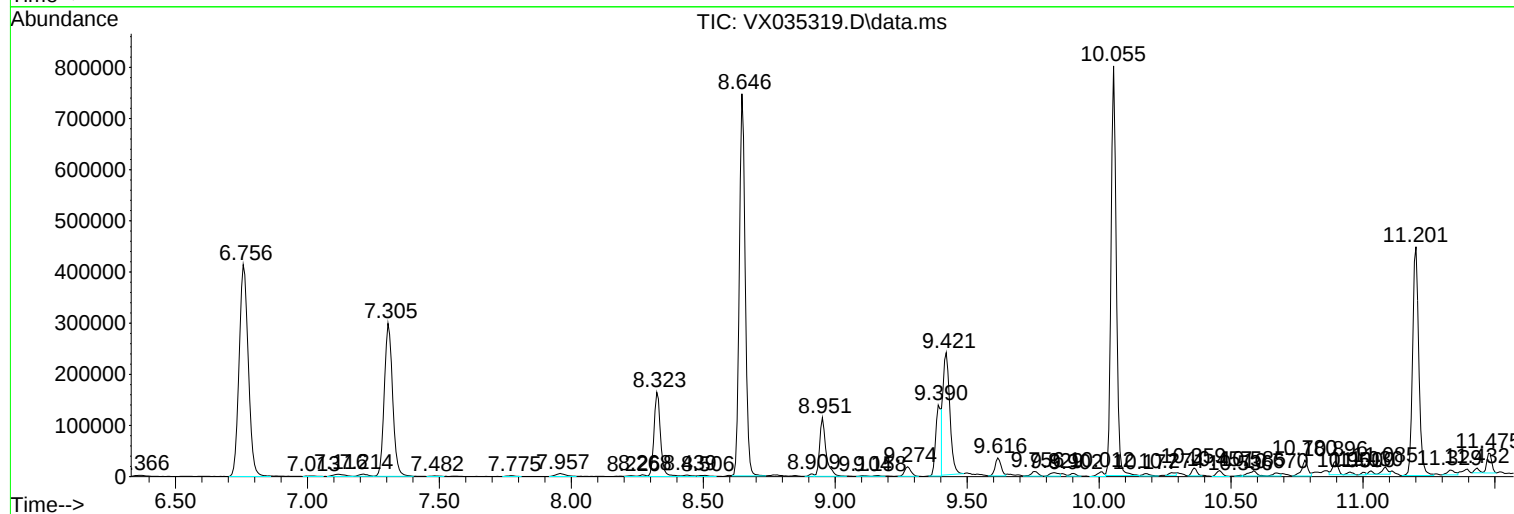
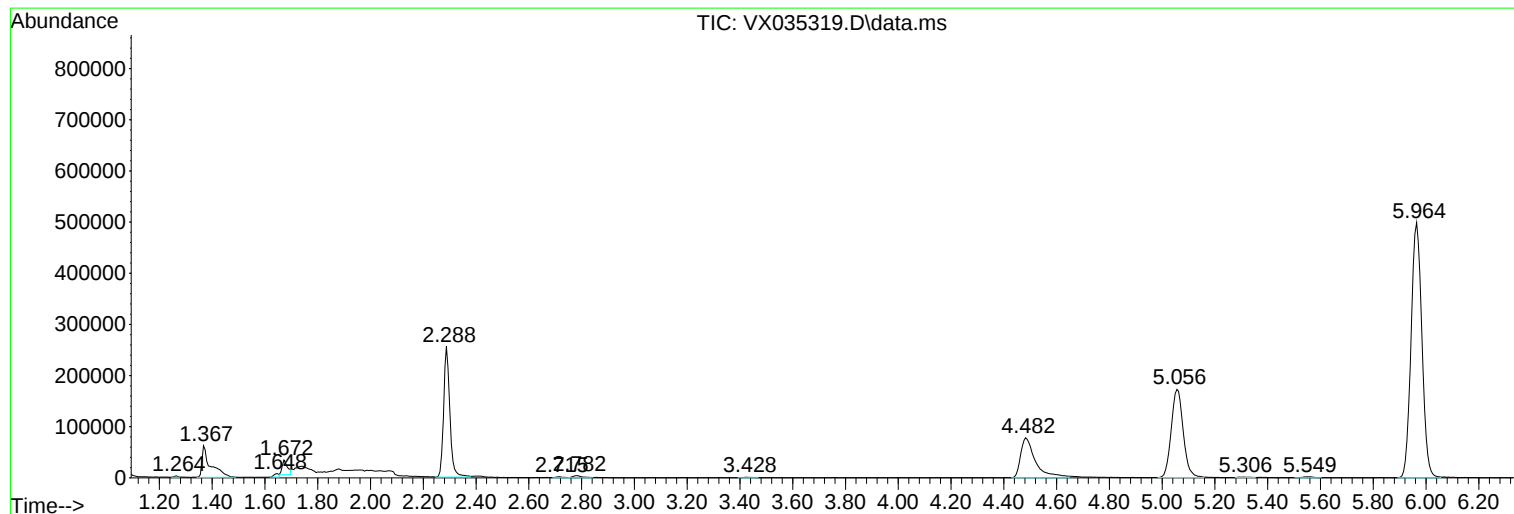
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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW953ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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



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Operator : JC/MD
Sample : 02479-12ME
Misc : 5.08g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

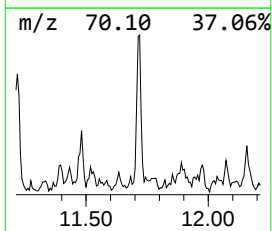
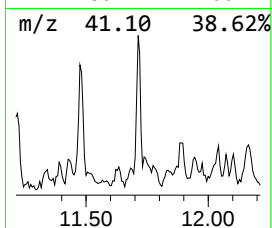
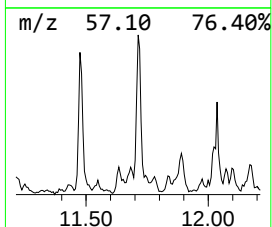
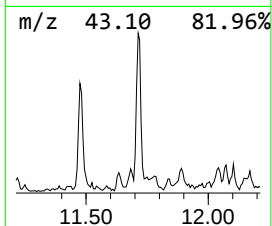
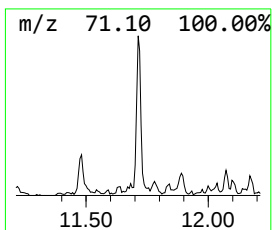
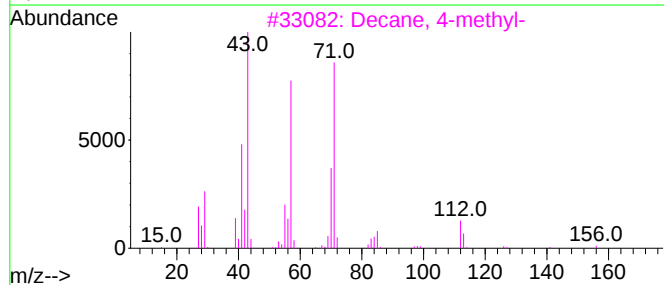
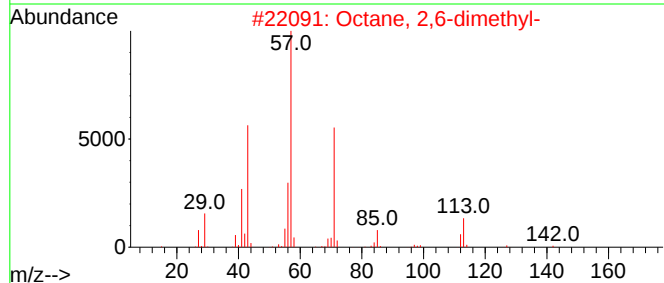
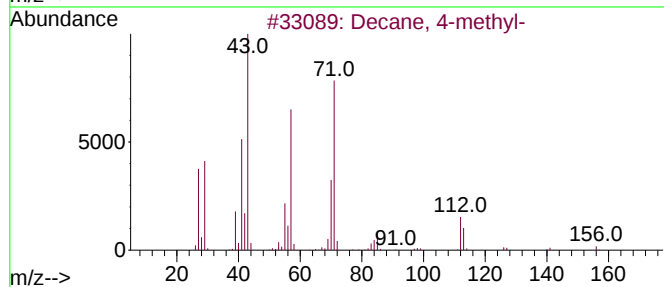
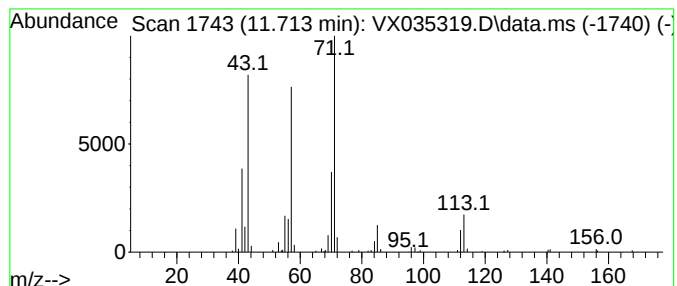
Instrument :
MSVOA_X
ClientSampleId :
EW953ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.713	3.13 ug/L	69541	1,4-Dichlorobenzene-d4		12.024	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Decane, 4-methyl-		156	C11H24	002847-72-5	87
2	Octane, 2,6-dimethyl-		142	C10H22	002051-30-1	86
3	Decane, 4-methyl-		156	C11H24	002847-72-5	80
4	Heptane, 3,3,5-trimethyl-		142	C10H22	007154-80-5	72
5	Heptane, 3,3,5-trimethyl-		142	C10H22	007154-80-5	72



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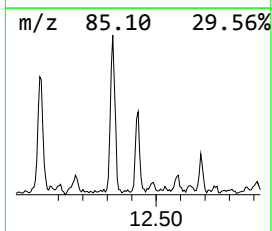
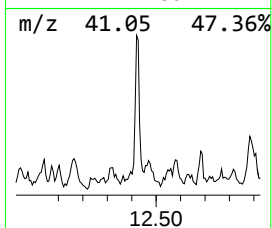
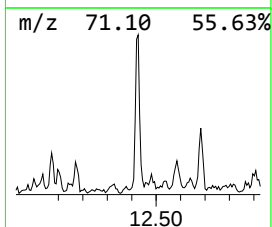
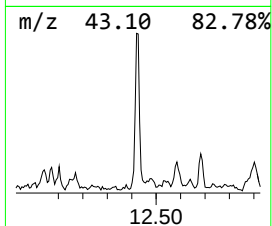
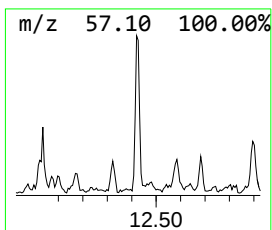
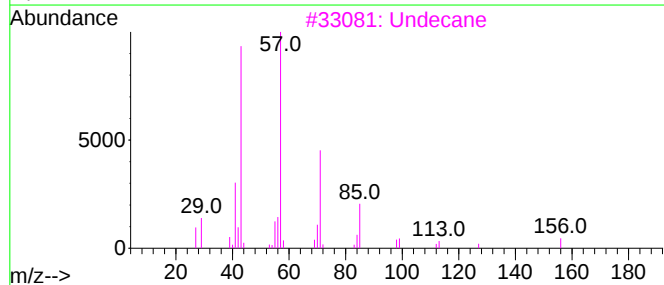
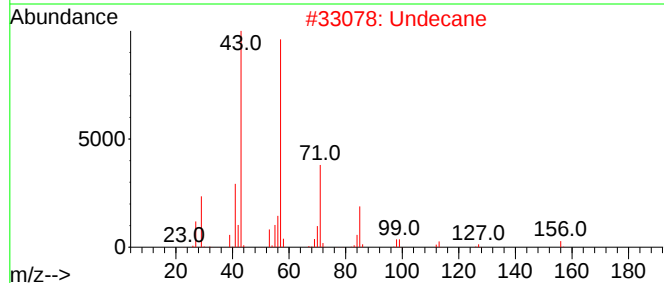
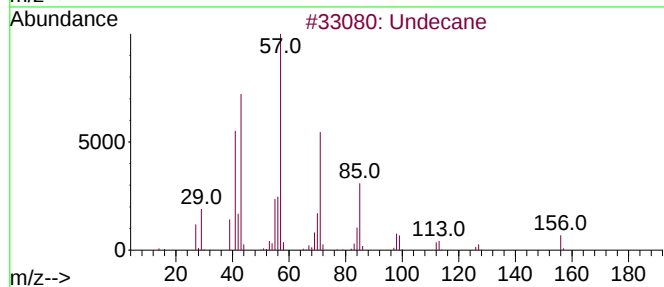
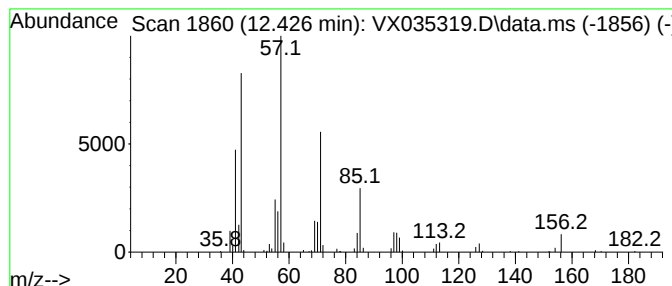
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041823WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.426	3.17 ug/L	70420	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	96
2	Undecane			156	C11H24	001120-21-4	87
3	Undecane			156	C11H24	001120-21-4	81
4	Carbonic acid, prop-1-en-2-yl tr...			284	C17H32O3	1000382-90-8	80
5	Dodecane			170	C12H26	000112-40-3	80



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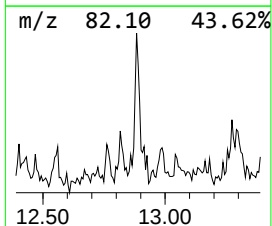
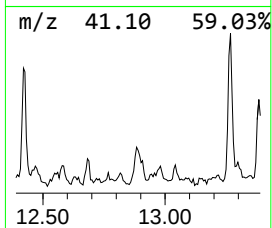
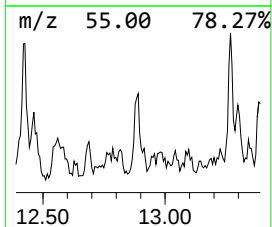
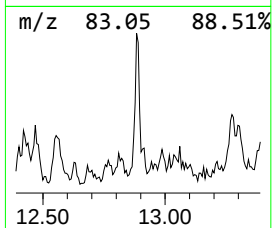
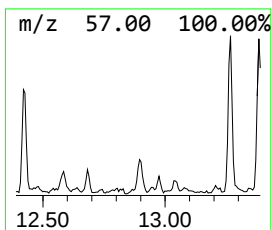
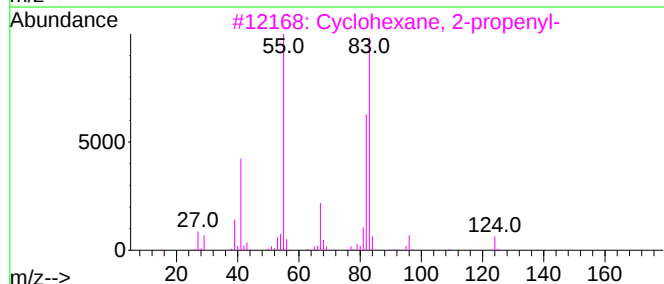
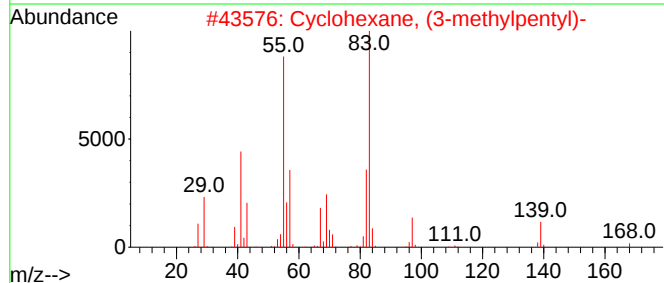
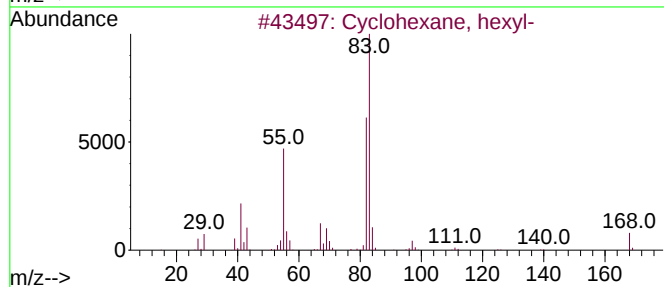
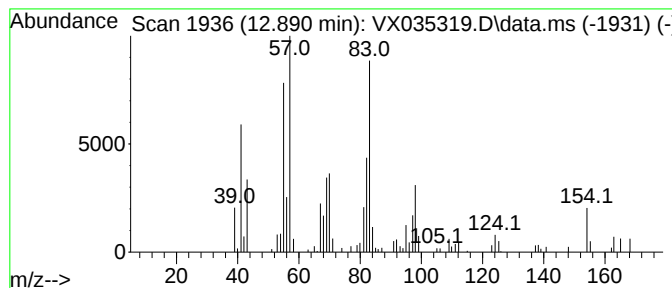
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Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Cyclic12.890 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.890	2.64 ug/L	58540	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, hexyl-	168	C12H24	004292-75-5	49
2			Cyclohexane, (3-methylpentyl)-	168	C12H24	061142-38-9	47
3			Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	46
4			Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	46
5			2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042623\
Data File : VX035319.D
Acq On : 26 Apr 2023 17:30
Operator : JC/MD
Sample : 02479-12ME
Misc : 5.08g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW953ME

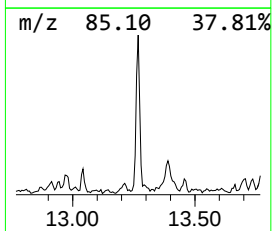
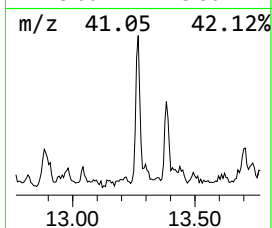
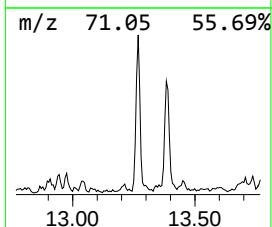
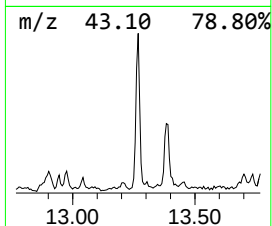
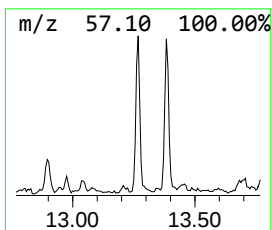
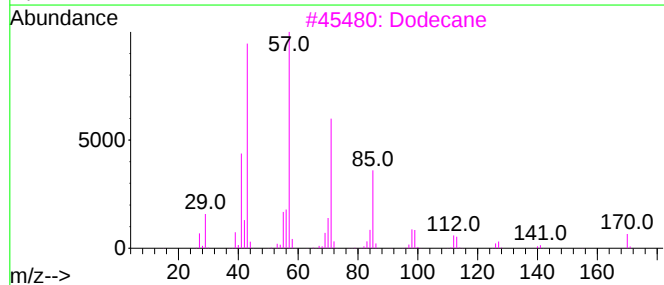
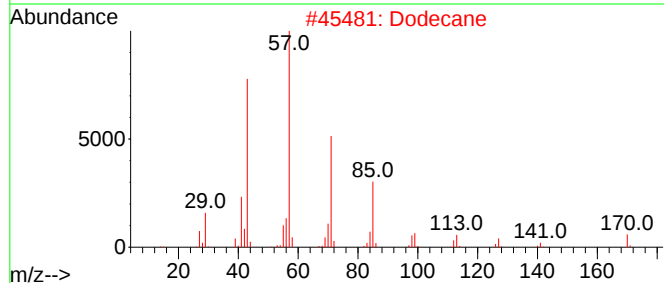
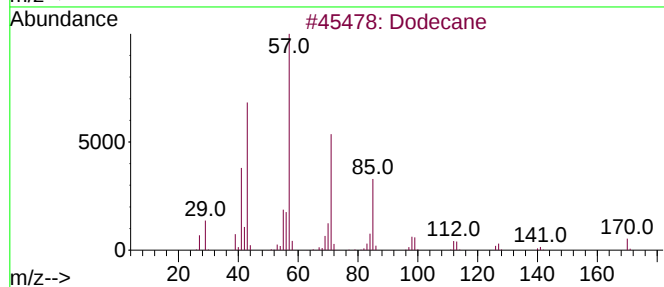
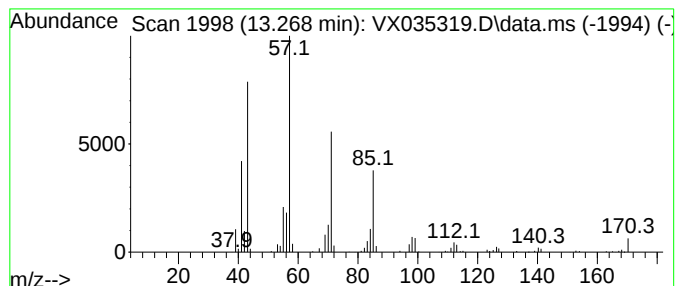
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Quant Title : VOC Analysis

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.268	5.09 ug/L	112953	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	97
2			Dodecane	170	C12H26	000112-40-3	93
3			Dodecane	170	C12H26	000112-40-3	87
4			Tetradecane	198	C14H30	000629-59-4	86
5			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042623\
Data File : VX035319.D
Acq On : 26 Apr 2023 17:30
Operator : JC/MD
Sample : 02479-12ME
Misc : 5.08g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW953ME

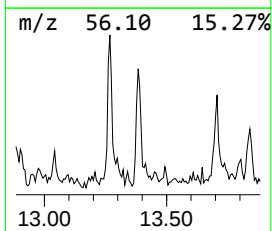
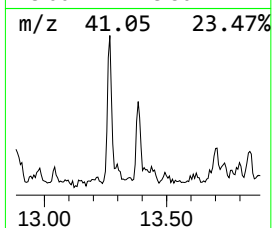
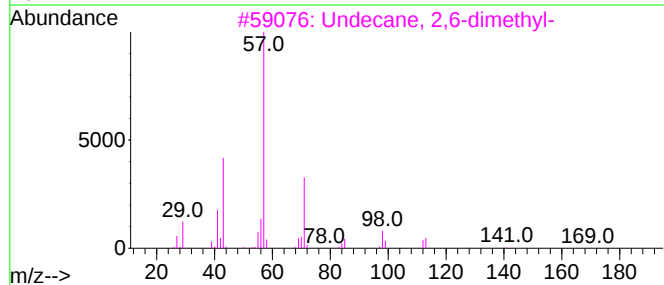
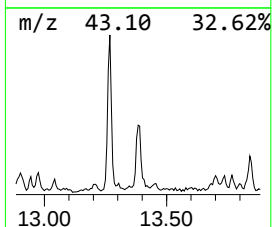
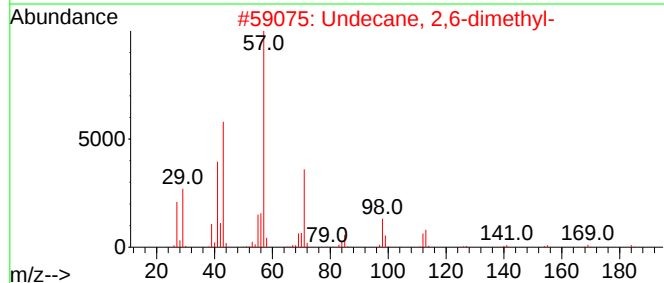
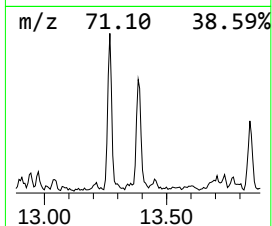
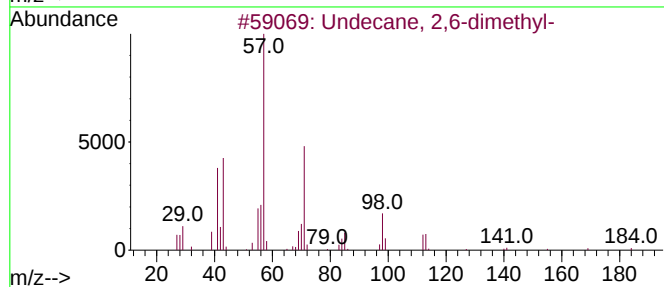
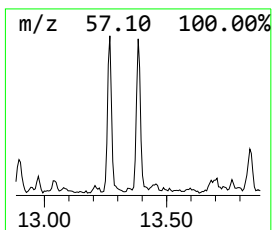
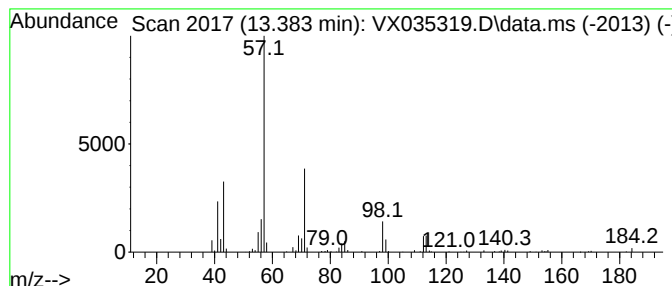
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Quant Title : VOC Analysis

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.383	3.43 ug/L	76016	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	91
2			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	91
3			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	90
4			Undecane, 5-ethyl-	184	C13H28	017453-94-0	72
5			Undecane, 2,5-dimethyl-	184	C13H28	017301-22-3	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042623\
Data File : VX035319.D
Acq On : 26 Apr 2023 17:30
Operator : JC/MD
Sample : 02479-12ME
Misc : 5.08g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW953ME

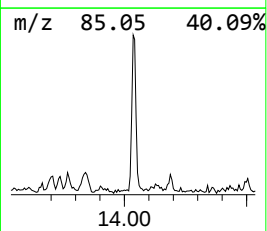
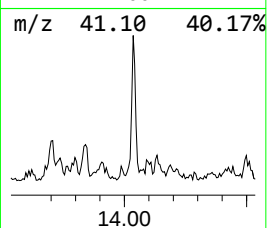
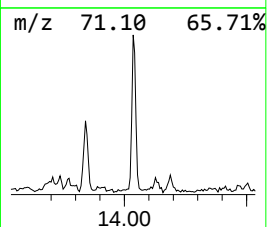
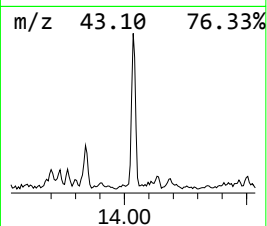
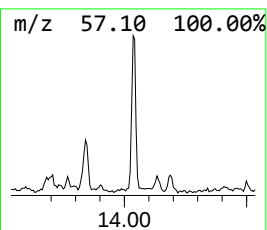
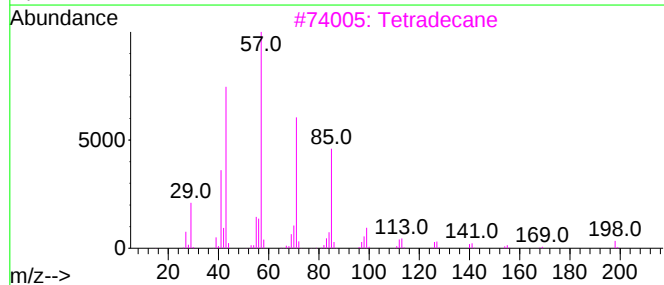
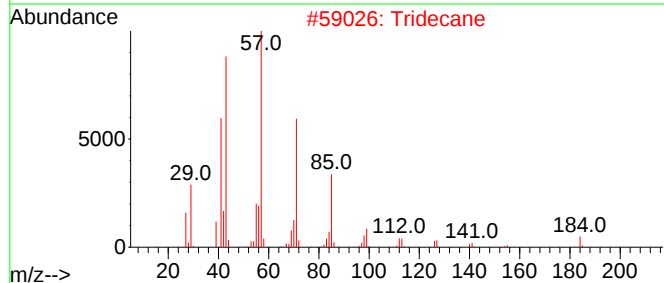
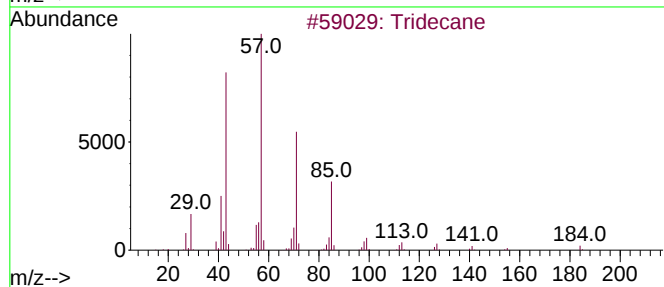
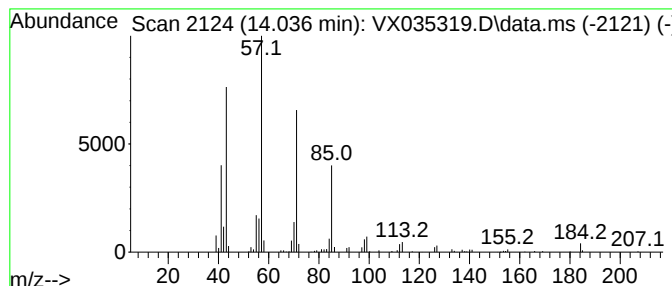
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Quant Title : VOC Analysis

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.036	3.79 ug/L	84100	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecane	184	C13H28	000629-50-5	96
2		Tridecane	184	C13H28	000629-50-5	94
3		Tetradecane	198	C14H30	000629-59-4	86
4		Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86
5		Nonadecane	268	C19H40	000629-92-5	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042623\
Data File : VX035319.D
Acq On : 26 Apr 2023 17:30
Operator : JC/MD
Sample : 02479-12ME
Misc : 5.08g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW953ME

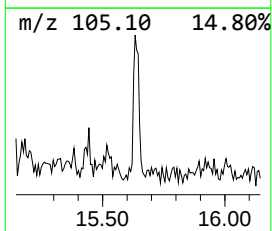
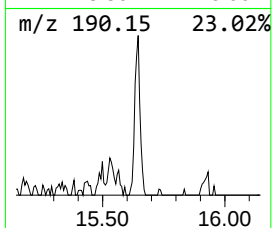
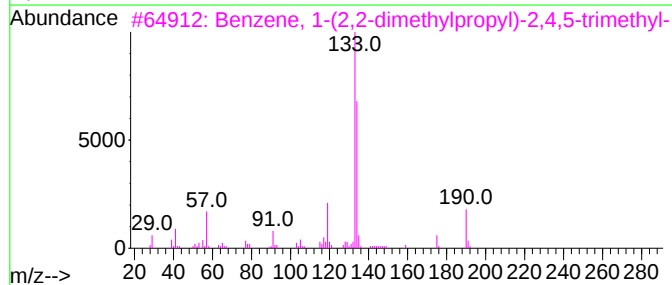
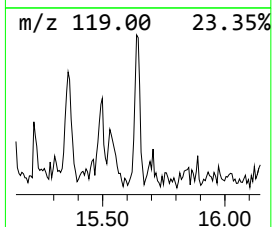
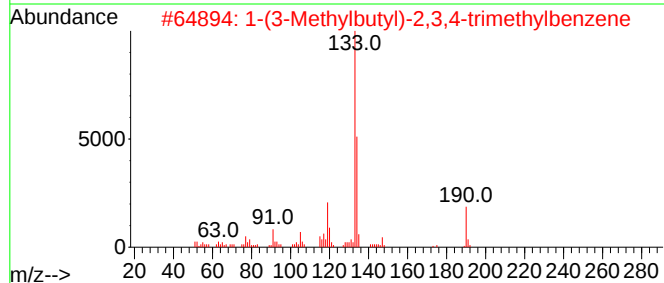
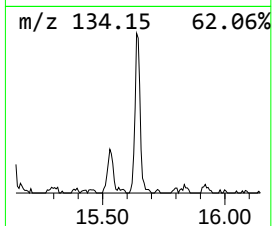
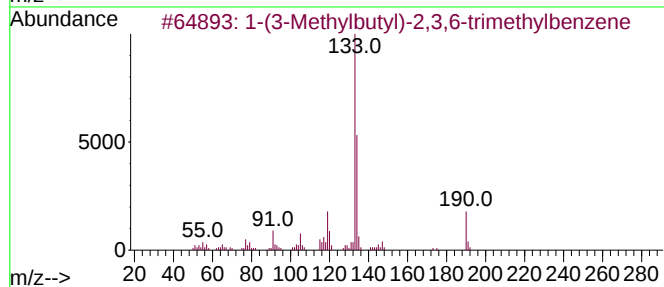
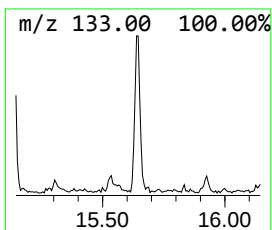
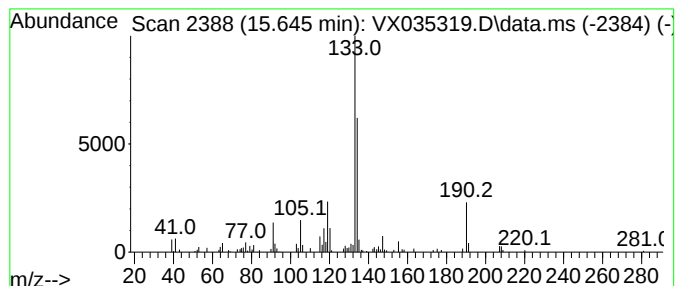
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Quant Title : VOC Analysis

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

Peak Number 8 1-(3-Methylbutyl)-2,3,6-tri... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.645	2.55 ug/L	56523	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-(3-Methylbutyl)-2,3,6-trimethy...	190	C14H22	084651-14-9	97
2			1-(3-Methylbutyl)-2,3,4-trimethy...	190	C14H22	107997-59-1	96
3			Benzene, 1-(2,2-dimethylpropyl)-...	190	C14H22	056666-87-6	87
4			Benzene, 1-isopentyl-2,4,5-trime...	190	C14H22	010425-90-8	76
5			2-Isopropenyl-3-methylpyrazine	134	C8H10N2	145984-65-2	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042623\
Data File : VX035319.D
Acq On : 26 Apr 2023 17:30
Operator : JC/MD
Sample : 02479-12ME
Misc : 5.08g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW953ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

						--Internal Standard--			
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(DEL) Alkane: S...	12.426	3.2	ug/L	70420	3	12.024	1109280	50.0	
(DEL) Alkane: C...	12.890	2.6	ug/L	58540	3	12.024	1109280	50.0	
(DEL) Alkane: S...	13.268	5.1	ug/L	112953	3	12.024	1109280	50.0	
(DEL) Alkane: S...	13.383	3.4	ug/L	76016	3	12.024	1109280	50.0	
(DEL) Alkane: S...	14.036	3.8	ug/L	84100	3	12.024	1109280	50.0	
1-(3-Methylbuty...	15.645	2.5	ug/L	56523	3	12.024	1109280	50.0	