

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061422\
 Data File : VX029496.D
 Acq On : 15 Jun 2022 03:22
 Operator : JC/MD
 Sample : N3226-18ME
 Misc : 6.26g/5mL/100uL/5.04mL/MSVOA_X/MEOH
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EW4N8ME

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\SFAMXML061322WMA.M
 Title : VOC Analysis

Signal : TIC: VX029496.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	7	9	14	rVB3	3346	3559	0.30%	0.035%
2	1.258	26	28	30	rBV	3805	3419	0.29%	0.034%
3	1.295	31	34	42	rVV3	6526	10845	0.92%	0.107%
4	1.368	42	46	57	rVB	96907	131849	11.16%	1.296%
5	1.636	87	90	92	rBV	18165	23213	1.96%	0.228%
6	1.666	92	95	102	rVB	46065	61184	5.18%	0.601%
7	2.282	188	196	205	rBV	199263	331715	28.08%	3.261%
8	2.380	207	212	213	rBV3	2284	3746	0.32%	0.037%
9	2.745	265	272	273	rBV4	3075	4438	0.38%	0.044%
10	2.953	296	306	319	rBV	19695	67885	5.75%	0.667%
11	3.422	377	383	390	rVV2	2098	4252	0.36%	0.042%
12	4.190	504	509	515	rVB3	877	2098	0.18%	0.021%
13	4.507	546	561	585	rBV	57748	307015	25.99%	3.018%
14	5.062	638	652	668	rVV	153329	485715	41.11%	4.775%
15	5.458	711	717	719	rBV4	1385	2579	0.22%	0.025%
16	5.611	735	742	743	rBV5	1451	2465	0.21%	0.024%
17	5.971	788	801	819	rBV2	411034	1181492	100.00%	11.614%
18	6.367	859	866	882	rBV5	6977	25626	2.17%	0.252%
19	6.605	899	905	912	rVB4	1324	2614	0.22%	0.026%
20	6.763	921	931	946	rBV	350288	842232	71.29%	8.279%
21	7.129	982	991	1001	rBV6	20345	52628	4.45%	0.517%
22	7.226	1001	1007	1012	rBV4	3164	7591	0.64%	0.075%
23	7.312	1012	1021	1040	rVB	242027	555426	47.01%	5.460%
24	7.482	1045	1049	1056	rVB4	1586	2715	0.23%	0.027%
25	7.556	1056	1061	1069	rVB4	1150	2495	0.21%	0.025%
26	7.775	1089	1097	1102	rBV3	4476	9293	0.79%	0.091%
27	7.964	1117	1128	1136	rBV6	5306	14557	1.23%	0.143%
28	8.226	1167	1171	1175	rBV5	1495	2657	0.22%	0.026%
29	8.330	1182	1188	1202	rBV	120816	208079	17.61%	2.045%
30	8.507	1211	1217	1221	rVB4	1906	3707	0.31%	0.036%
31	8.653	1225	1241	1248	rBV	558356	899321	76.12%	8.841%
32	8.720	1248	1252	1258	rVB2	15226	24031	2.03%	0.236%
33	8.909	1280	1283	1286	rBV4	2478	3823	0.32%	0.038%
34	8.958	1286	1291	1305	rVB	81402	136689	11.57%	1.344%
35	9.110	1310	1316	1321	rVV6	3031	4731	0.40%	0.047%
36	9.269	1339	1342	1348	rBV6	2550	4860	0.41%	0.048%

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 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EW4N8ME

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\SFAMXML061322WMA.M
 Title : VOC Analysis

37	9.397	1356	1363	1377	rBV	291447	668173	56.55%	6.568%
38	9.500	1377	1380	1384	rBV4	1792	2976	0.25%	0.029%
39	9.616	1394	1399	1403	rBV2	7352	11444	0.97%	0.112%
40	9.653	1403	1405	1410	rVV5	1929	2746	0.23%	0.027%
41	9.830	1428	1434	1441	rBV6	3171	6195	0.52%	0.061%
42	9.903	1443	1446	1454	rVB3	3209	5056	0.43%	0.050%
43	10.012	1454	1464	1466	rBV3	3234	5328	0.45%	0.052%
44	10.055	1466	1471	1481	rVV	694311	937249	79.33%	9.213%
45	10.201	1487	1495	1498	rBV2	3967	6392	0.54%	0.063%
46	10.305	1502	1512	1517	rBV4	10705	21885	1.85%	0.215%
47	10.360	1517	1521	1528	rVB2	7353	11308	0.96%	0.111%
48	10.458	1533	1537	1543	rVB4	3614	5135	0.43%	0.050%
49	10.592	1552	1559	1564	rBV8	3213	6700	0.57%	0.066%
50	10.647	1564	1568	1576	rVV	8009	13043	1.10%	0.128%
51	10.781	1582	1590	1594	rBV3	10310	15330	1.30%	0.151%
52	10.860	1599	1603	1605	rVV3	2712	3425	0.29%	0.034%
53	10.896	1605	1609	1614	rVB3	6075	9738	0.82%	0.096%
54	10.957	1616	1619	1623	rBV5	2699	4459	0.38%	0.044%
55	11.031	1629	1631	1635	rVB2	2660	2590	0.22%	0.025%
56	11.085	1635	1640	1642	rBV3	5722	7934	0.67%	0.078%
57	11.110	1642	1644	1650	rVB5	5987	9228	0.78%	0.091%
58	11.195	1650	1658	1668	rBV	451752	620832	52.55%	6.103%
59	11.390	1685	1690	1694	rBV6	4592	7610	0.64%	0.075%
60	11.433	1694	1697	1699	rVV2	4045	4889	0.41%	0.048%
61	11.476	1701	1704	1710	rVB	21825	29460	2.49%	0.290%
62	11.634	1724	1730	1734	rBV6	4650	9743	0.82%	0.096%
63	11.683	1734	1738	1740	rBV4	2967	4009	0.34%	0.039%
64	11.713	1740	1743	1747	rVV	15678	19019	1.61%	0.187%
65	11.756	1747	1750	1759	rVB2	11220	20295	1.72%	0.200%
66	11.854	1759	1766	1767	rBV5	3209	6358	0.54%	0.063%
67	11.896	1769	1773	1777	rVB4	7076	9749	0.83%	0.096%
68	11.945	1777	1781	1783	rBV5	3576	4889	0.41%	0.048%
69	11.976	1783	1786	1788	rVB4	2939	3198	0.27%	0.031%
70	12.024	1789	1794	1800	rBV	762099	924603	78.26%	9.089%
71	12.079	1800	1803	1804	rBV3	3141	3422	0.29%	0.034%
72	12.177	1812	1819	1826	rVB5	6484	13459	1.14%	0.132%
73	12.244	1826	1830	1833	rBV5	2728	4577	0.39%	0.045%
74	12.323	1838	1843	1849	rVV	635816	802953	67.96%	7.893%
75	12.427	1856	1860	1864	rVB	39682	44751	3.79%	0.440%
76	12.475	1864	1868	1873	rVB7	4493	8466	0.72%	0.083%

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 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EW4N8ME

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

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

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML061322WMA.M
 Title : VOC Analysis

77	12.561	1876	1882	1883	rBV5	3491	6233	0.53%	0.061%
78	12.585	1883	1886	1890	rVB5	4331	5836	0.49%	0.057%
79	12.683	1898	1902	1906	rBV5	5554	8674	0.73%	0.085%
80	12.768	1913	1916	1918	rBV3	2974	3246	0.27%	0.032%
81	12.896	1932	1937	1943	rBV5	7485	20607	1.74%	0.203%
82	12.975	1947	1950	1955	rVV6	7785	11340	0.96%	0.111%
83	13.042	1958	1961	1965	rVB6	5305	6660	0.56%	0.065%
84	13.146	1974	1978	1982	rBV5	2092	4186	0.35%	0.041%
85	13.207	1986	1988	1992	rBV5	2396	2704	0.23%	0.027%
86	13.268	1994	1998	2001	rBV	51562	57534	4.87%	0.566%
87	13.384	2014	2017	2021	rBV	29498	36554	3.09%	0.359%
88	13.701	2067	2069	2072	rVB3	4855	4347	0.37%	0.043%
89	13.780	2078	2082	2088	rVV	22801	38099	3.22%	0.375%
90	13.847	2088	2093	2098	rVB	16801	22787	1.93%	0.224%
91	14.042	2121	2125	2132	rBV	45195	53124	4.50%	0.522%
92	14.103	2132	2135	2137	rVV3	5133	5675	0.48%	0.056%
93	14.134	2138	2140	2143	rVB3	7348	7634	0.65%	0.075%
94	14.189	2147	2149	2152	rVB4	4388	4423	0.37%	0.043%
95	14.615	2215	2219	2220	rBV	13314	13921	1.18%	0.137%
96	14.640	2220	2223	2226	rVB	21325	25870	2.19%	0.254%
97	14.756	2238	2242	2245	rBV	36242	47125	3.99%	0.463%
98	15.213	2314	2317	2321	rVB3	13434	16086	1.36%	0.158%
99	15.493	2357	2363	2367	rBV4	18210	30064	2.54%	0.296%
100	16.383	2502	2509	2515	rBV9	4354	10795	0.91%	0.106%

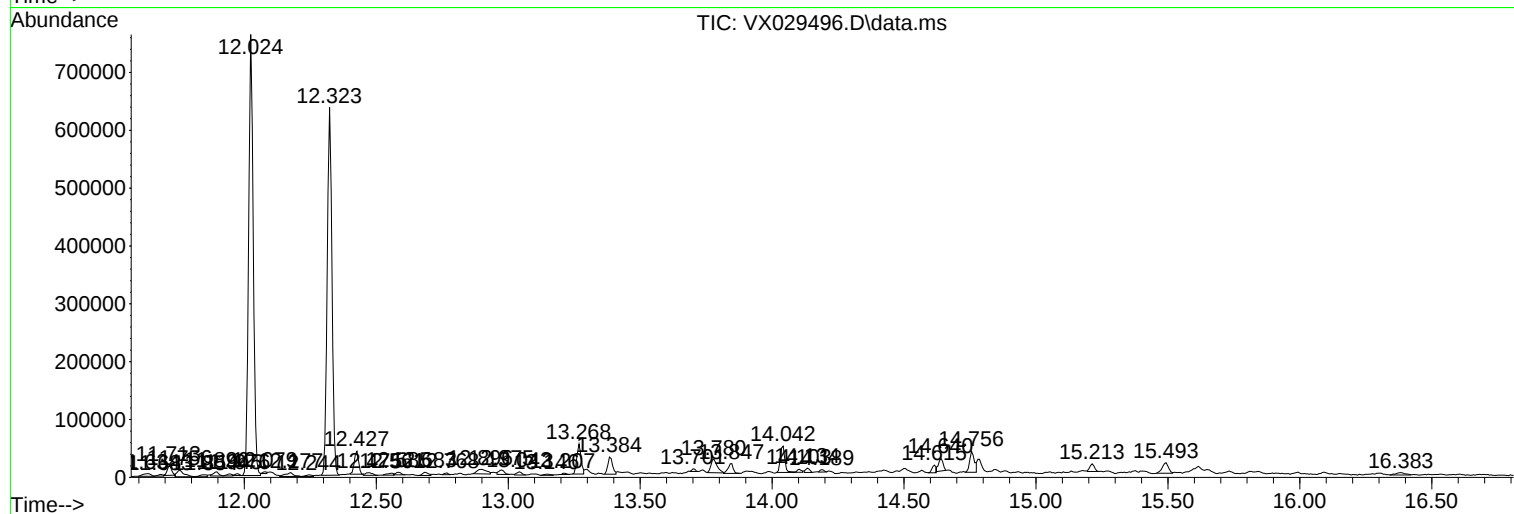
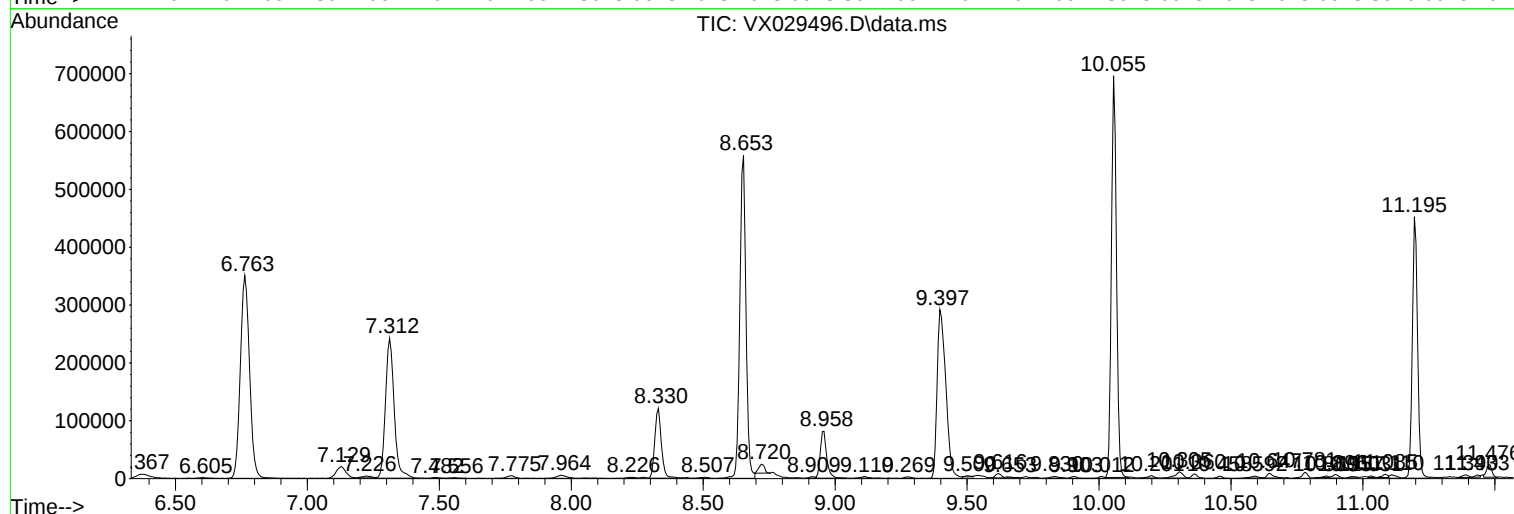
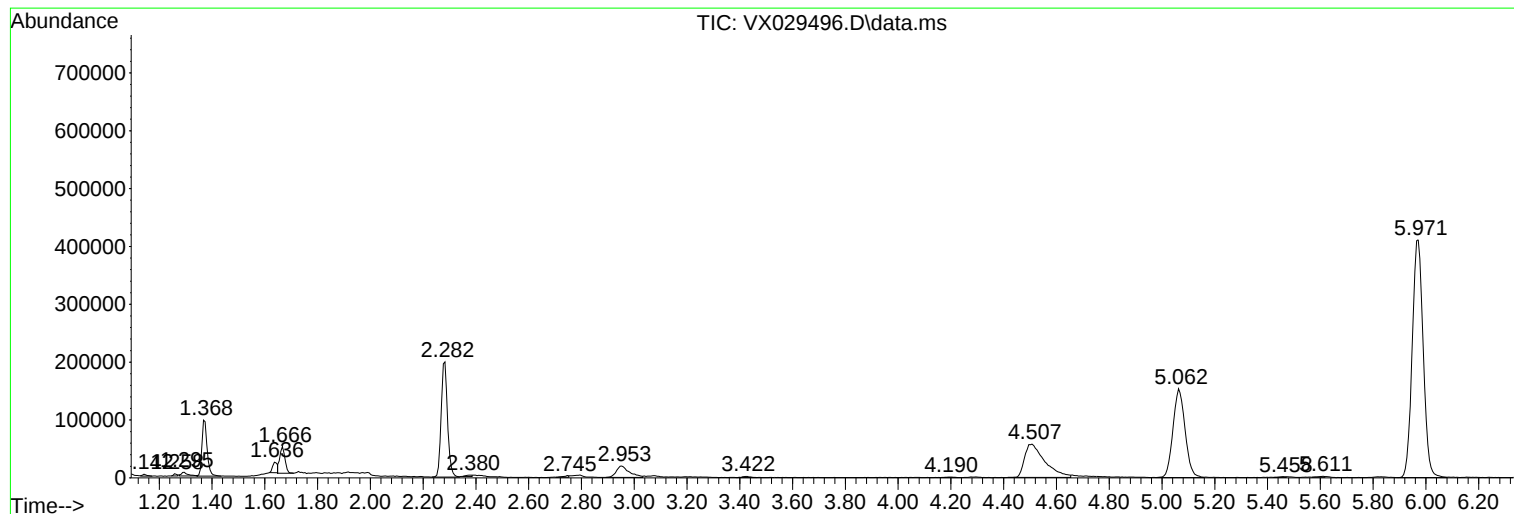
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Misc : 6.26g/5mL/100uL/5.04mL/MSVOA_X/MEOH
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW4N8ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML061322WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061422\
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Acq On : 15 Jun 2022 03:22
Operator : JC/MD
Sample : N3226-18ME
Misc : 6.26g/5mL/100uL/5.04mL/MSVOA_X/MEOH
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW4N8ME

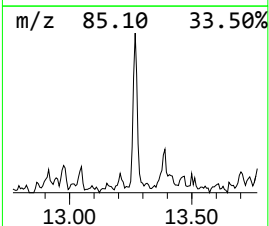
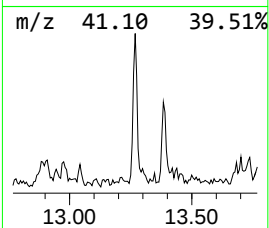
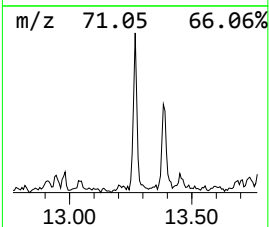
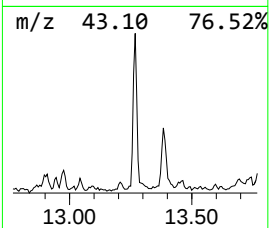
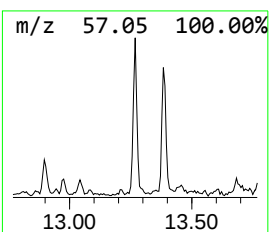
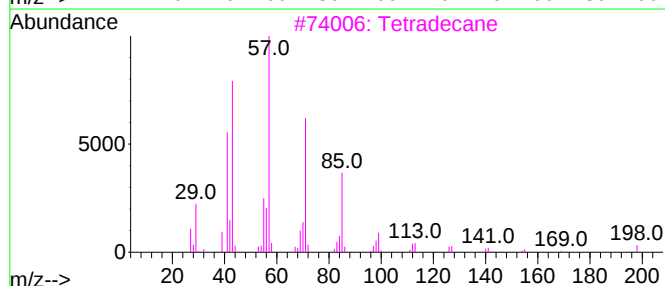
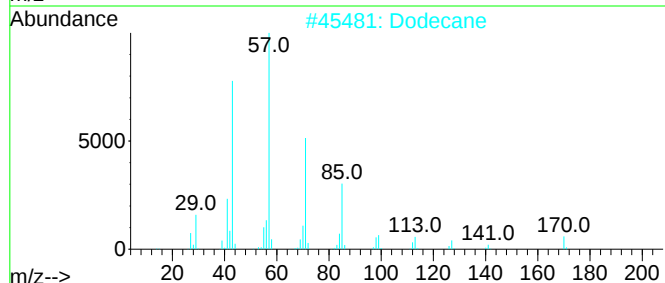
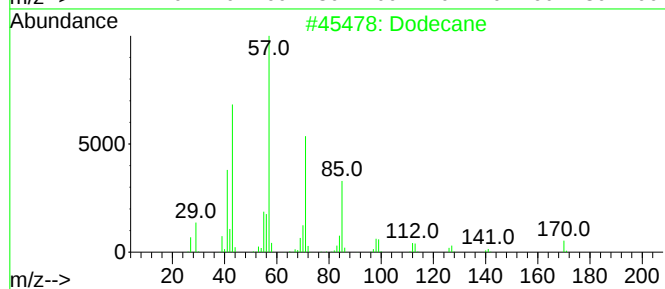
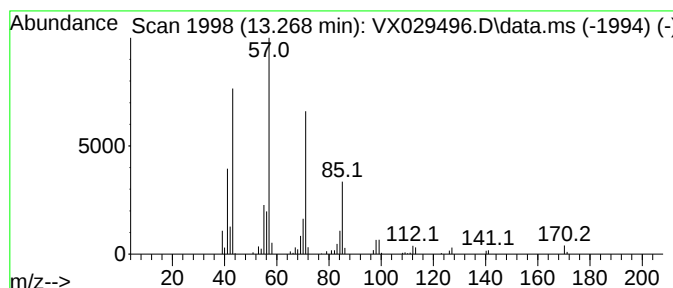
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML061322WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.268	3.11 ug/L	57534	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	94
2			Dodecane	170	C12H26	000112-40-3	91
3			Tetradecane	198	C14H30	000629-59-4	90
4			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	90
5			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	90



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Sample : N3226-18ME
Misc : 6.26g/5mL/100uL/5.04mL/MSVOA_X/MEOH
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW4N8ME

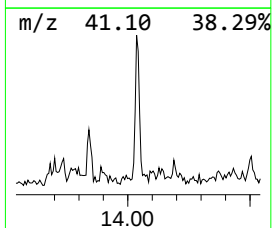
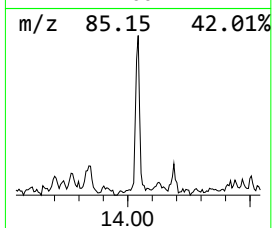
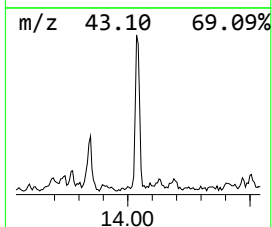
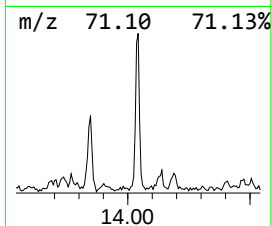
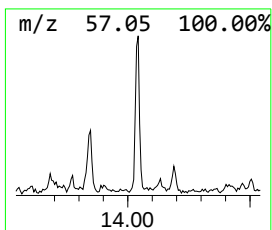
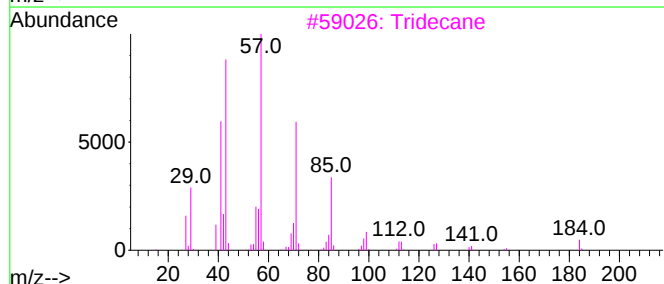
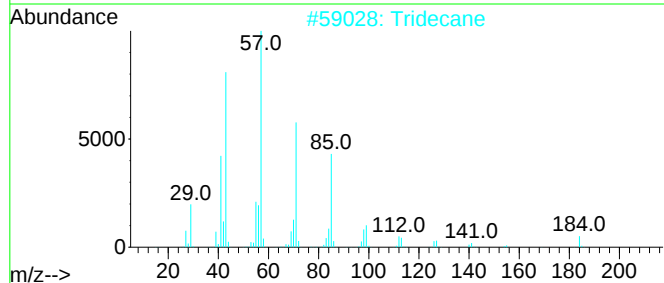
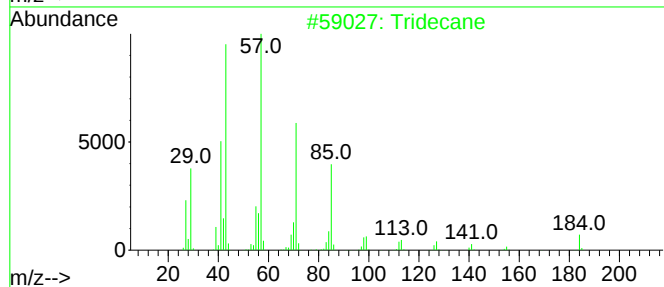
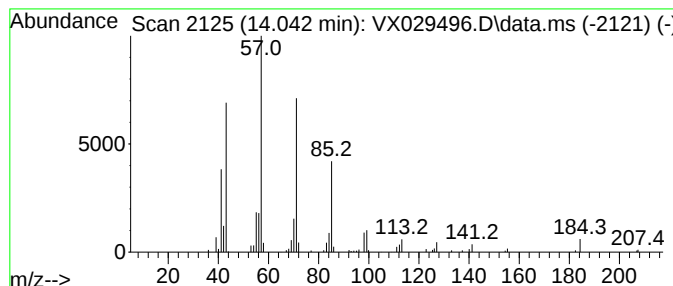
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML061322WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.042	2.87 ug/L	53124	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	94
2			Tridecane	184	C13H28	000629-50-5	94
3			Tridecane	184	C13H28	000629-50-5	94
4			Tridecane	184	C13H28	000629-50-5	91
5			Sulfurous acid, 2-propyl tetra...	320	C17H36O3S	1010309-12-5	90



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Misc : 6.26g/5mL/100uL/5.04mL/MSVOA_X/MEOH
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW4N8ME

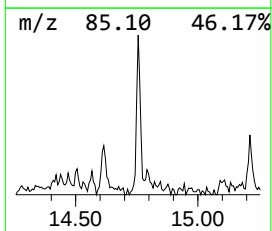
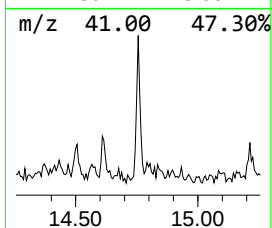
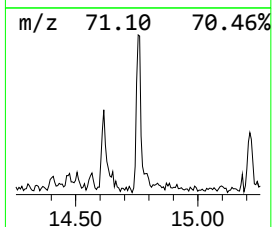
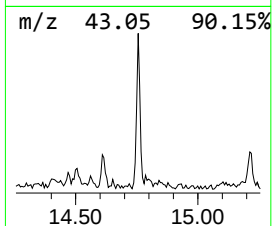
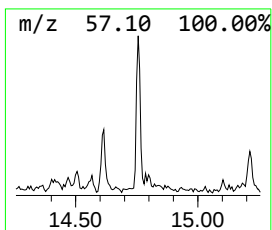
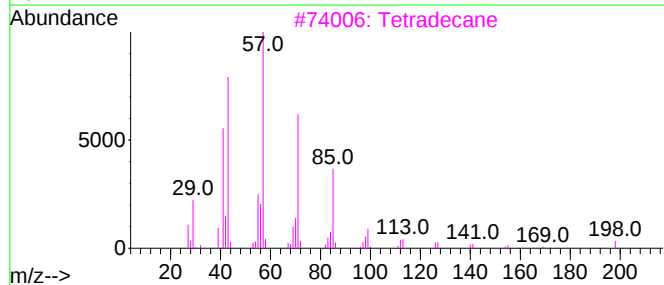
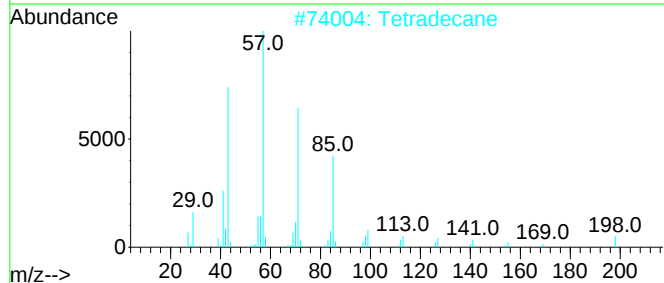
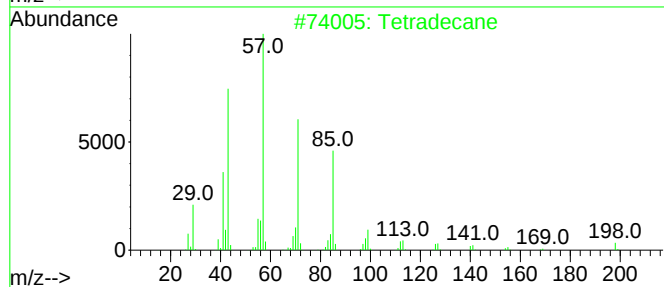
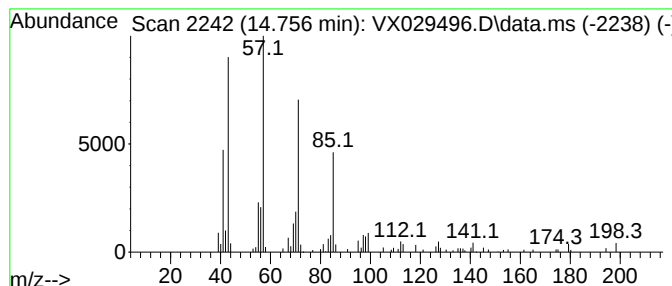
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML061322WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.756	2.55 ug/L	47125	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	95
2			Tetradecane	198	C14H30	000629-59-4	91
3			Tetradecane	198	C14H30	000629-59-4	91
4			Tridecane	184	C13H28	000629-50-5	86
5			Tridecane	184	C13H28	000629-50-5	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061422\
Data File : VX029496.D
Acq On : 15 Jun 2022 03:22
Operator : JC/MD
Sample : N3226-18ME
Misc : 6.26g/5mL/100uL/5.04mL/MSVOA_X/MEOH
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW4N8ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML061322WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	13.268	3.1	ug/L	57534	3	12.024	924603	50.0
(DEL) Alkane: S...	14.042	2.9	ug/L	53124	3	12.024	924603	50.0
(DEL) Alkane: S...	14.756	2.5	ug/L	47125	3	12.024	924603	50.0