

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121324\
 Data File : VX044297.D
 Acq On : 13 Dec 2024 21:17
 Operator : JC/MD
 Sample : P5153-03ME
 Misc : 3.98g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E28P1ME

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\SFAMXLM120524WMA.M
 Title : VOC Analysis

Signal : TIC: VX044297.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	22	29	34	rBV3	11778	17217	2.42%	0.299%
2	1.367	43	46	49	rBV	34924	45272	6.35%	0.786%
3	1.629	68	89	95	rBV2	71292	250300	35.12%	4.347%
4	2.129	169	171	176	rVB5	2909	4364	0.61%	0.076%
5	2.276	188	195	207	rBV	118779	189741	26.63%	3.295%
6	2.782	273	278	280	rBV3	889	1253	0.18%	0.022%
7	2.940	298	304	311	rBV3	4739	11984	1.68%	0.208%
8	3.227	347	351	355	rBV3	715	1057	0.15%	0.018%
9	3.422	377	383	389	rVV5	3207	7097	1.00%	0.123%
10	3.696	423	428	431	rBV3	515	809	0.11%	0.014%
11	4.416	541	546	548	rVB3	426	817	0.11%	0.014%
12	4.489	548	558	582	rBV2	28325	126209	17.71%	2.192%
13	4.739	596	599	602	rVV3	607	745	0.10%	0.013%
14	5.050	639	650	668	rBV	95092	290775	40.80%	5.050%
15	5.501	721	724	725	rBV2	788	747	0.10%	0.013%
16	5.678	751	753	756	rBV4	678	895	0.13%	0.016%
17	5.812	773	775	779	rVB3	568	724	0.10%	0.013%
18	5.958	788	799	815	rBV2	246688	712619	100.00%	12.377%
19	6.080	817	819	821	rVV2	1149	1121	0.16%	0.019%
20	6.104	821	823	825	rVB2	809	861	0.12%	0.015%
21	6.366	864	866	867	rVV2	1123	1072	0.15%	0.019%
22	6.391	868	870	872	rVV2	1465	1409	0.20%	0.024%
23	6.568	895	899	900	rBV3	975	1024	0.14%	0.018%
24	6.592	900	903	905	rBV2	570	793	0.11%	0.014%
25	6.757	921	930	946	rBV	200217	500202	70.19%	8.688%
26	7.061	978	980	983	rBV2	732	900	0.13%	0.016%
27	7.110	983	988	990	rBV4	1655	2592	0.36%	0.045%
28	7.202	1001	1003	1004	rBV2	792	773	0.11%	0.013%
29	7.226	1004	1007	1010	rVV4	1545	2346	0.33%	0.041%
30	7.305	1010	1020	1039	rVB	141414	326483	45.81%	5.670%
31	7.952	1121	1126	1127	rBV3	1313	1578	0.22%	0.027%
32	8.031	1136	1139	1142	rBV3	864	1279	0.18%	0.022%
33	8.073	1144	1146	1149	rVV2	549	690	0.10%	0.012%
34	8.110	1149	1152	1155	rVB3	839	1003	0.14%	0.017%
35	8.268	1175	1178	1181	rVV4	1258	1531	0.21%	0.027%
36	8.323	1181	1187	1202	rVV	79463	133541	18.74%	2.319%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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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\SFAMXLM120524WMA.M
 Title : VOC Analysis

37	8.427	1202	1204	1207	rVB4	1011	1086	0.15%	0.019%
38	8.646	1233	1240	1254	rBV	327489	528192	74.12%	9.174%
39	8.909	1280	1283	1285	rBV3	655	867	0.12%	0.015%
40	8.951	1285	1290	1302	rVB	50440	85897	12.05%	1.492%
41	9.213	1328	1333	1336	rBV3	650	1153	0.16%	0.020%
42	9.281	1341	1344	1348	rVB4	701	983	0.14%	0.017%
43	9.396	1357	1363	1382	rBV	130467	267083	37.48%	4.639%
44	9.616	1394	1399	1404	rVB4	2419	4290	0.60%	0.075%
45	9.707	1409	1414	1419	rBV6	1369	2964	0.42%	0.051%
46	9.756	1420	1422	1428	rVB5	836	1376	0.19%	0.024%
47	9.829	1432	1434	1437	rBV4	515	725	0.10%	0.013%
48	9.854	1437	1438	1442	rVV2	738	756	0.11%	0.013%
49	9.902	1442	1446	1448	rVB2	1715	1709	0.24%	0.030%
50	10.006	1460	1463	1465	rVV4	1046	1639	0.23%	0.028%
51	10.055	1465	1471	1487	rVV	412399	597519	83.85%	10.378%
52	10.250	1500	1503	1504	rVV	822	810	0.11%	0.014%
53	10.268	1504	1506	1509	rVV3	1211	1265	0.18%	0.022%
54	10.311	1509	1513	1517	rVV6	819	1429	0.20%	0.025%
55	10.360	1517	1521	1526	rVB3	2957	4188	0.59%	0.073%
56	10.512	1544	1546	1549	rBV3	838	840	0.12%	0.015%
57	10.780	1587	1590	1594	rVB3	2308	2503	0.35%	0.043%
58	10.860	1600	1603	1605	rVV3	911	1385	0.19%	0.024%
59	10.896	1605	1609	1613	rVB3	1990	2663	0.37%	0.046%
60	11.024	1626	1630	1632	rVB4	950	1051	0.15%	0.018%
61	11.085	1637	1640	1642	rVB3	1806	1749	0.25%	0.030%
62	11.109	1642	1644	1648	rVB3	1249	1303	0.18%	0.023%
63	11.189	1651	1657	1666	rBV	236723	319657	44.86%	5.552%
64	11.329	1677	1680	1682	rVV2	1362	1594	0.22%	0.028%
65	11.390	1687	1690	1694	rVB3	904	1114	0.16%	0.019%
66	11.426	1694	1696	1697	rBV2	1455	1218	0.17%	0.021%
67	11.475	1700	1704	1710	rVV3	6736	8884	1.25%	0.154%
68	11.591	1720	1723	1725	rBV2	738	793	0.11%	0.014%
69	11.628	1725	1729	1734	rBV5	1218	2196	0.31%	0.038%
70	11.683	1734	1738	1740	rBV5	1100	1777	0.25%	0.031%
71	11.713	1740	1743	1746	rBV2	6175	7104	1.00%	0.123%
72	11.744	1746	1748	1752	rVB4	1187	1230	0.17%	0.021%
73	11.884	1769	1771	1775	rBV3	2423	2789	0.39%	0.048%
74	12.024	1788	1794	1800	rBV	384663	521147	73.13%	9.051%
75	12.152	1812	1815	1816	rBV3	1405	1581	0.22%	0.027%
76	12.317	1837	1842	1853	rBV	360266	456735	64.09%	7.933%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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Max Peaks: 100

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120524WMA.M
 Title : VOC Analysis

77	12.420	1855	1859	1864	rBV	20038	25025	3.51%	0.435%
78	12.573	1882	1884	1885	rBV2	1930	1460	0.20%	0.025%
79	12.682	1898	1902	1906	rVB6	3455	4671	0.66%	0.081%
80	12.896	1930	1937	1942	rBV9	5894	13614	1.91%	0.236%
81	12.945	1942	1945	1947	rVV4	2750	3117	0.44%	0.054%
82	12.969	1947	1949	1954	rVV4	3701	4854	0.68%	0.084%
83	13.036	1957	1960	1966	rVV6	3242	4258	0.60%	0.074%
84	13.268	1994	1998	2007	rVB	29772	43290	6.07%	0.752%
85	13.341	2007	2010	2013	rBV5	2472	3169	0.44%	0.055%
86	13.383	2013	2017	2020	rBV	18234	21405	3.00%	0.372%
87	13.700	2067	2069	2071	rBV2	4546	3612	0.51%	0.063%
88	13.841	2088	2092	2096	rVB3	10614	13739	1.93%	0.239%
89	13.981	2114	2115	2119	rBV5	2386	2786	0.39%	0.048%
90	14.036	2120	2124	2132	rVV	30421	36175	5.08%	0.628%
91	14.097	2132	2134	2137	rBV3	3723	4098	0.58%	0.071%
92	14.493	2197	2199	2206	rVB8	4786	9345	1.31%	0.162%
93	14.609	2215	2218	2223	rBV2	8358	11046	1.55%	0.192%
94	14.755	2238	2242	2246	rBV	23215	27580	3.87%	0.479%
95	15.212	2313	2317	2324	rVB5	8371	13481	1.89%	0.234%
96	15.365	2340	2342	2344	rBV3	2703	2502	0.35%	0.043%
97	15.487	2359	2362	2367	rVB2	11816	15130	2.12%	0.263%
98	15.706	2395	2398	2400	rBV4	1659	1765	0.25%	0.031%
99	16.371	2503	2507	2510	rBV5	4180	5644	0.79%	0.098%
100	16.724	2563	2565	2566	rVB2	1412	763	0.11%	0.013%

Sum of corrected areas: 5757596

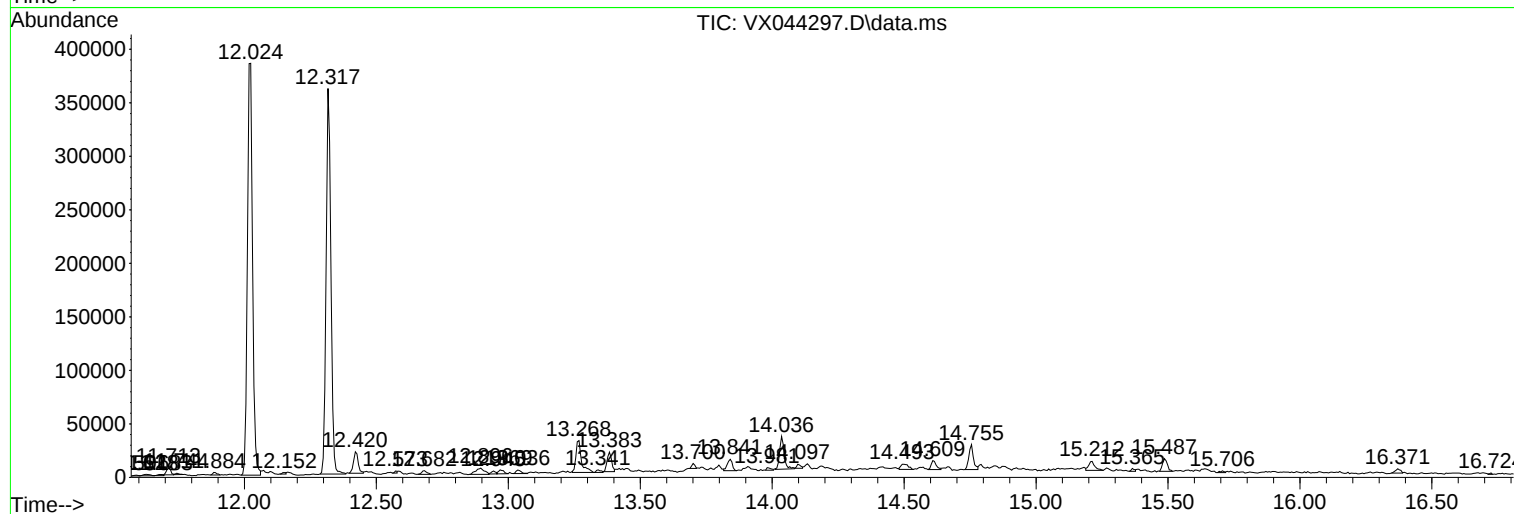
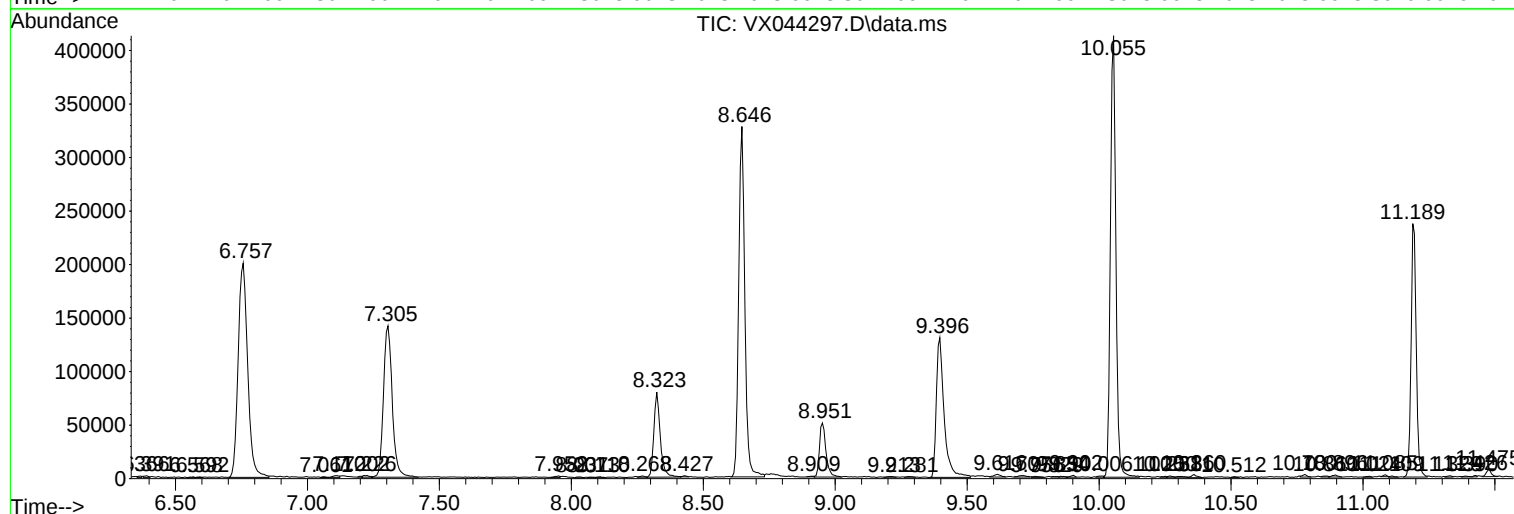
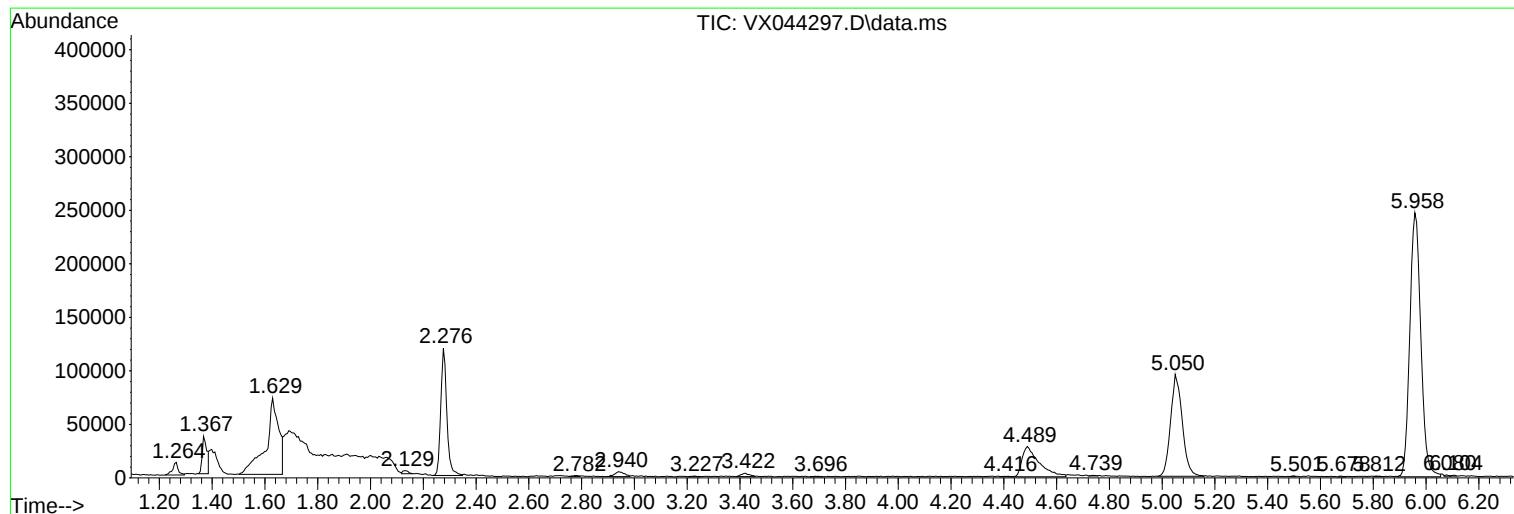
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ALS Vial : 32 Sample Multiplier: 1

Instrument :
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ClientSampleId :
E28P1ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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Instrument :
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ClientSampleId :
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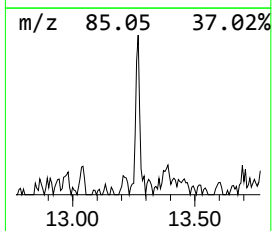
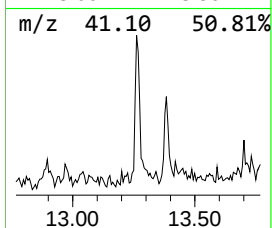
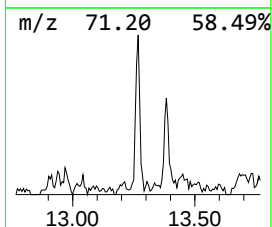
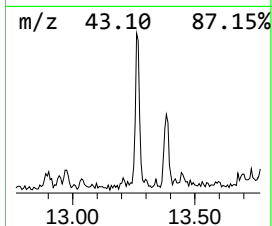
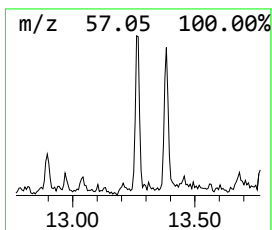
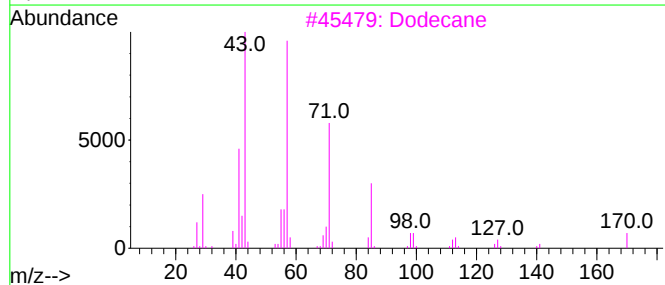
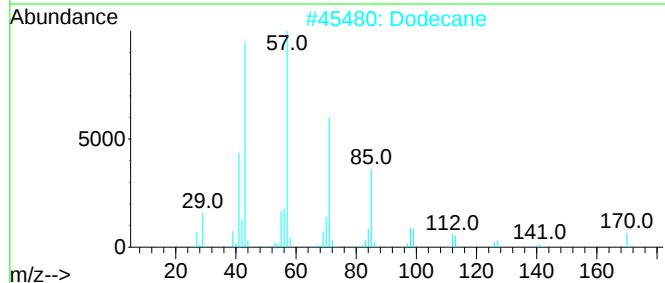
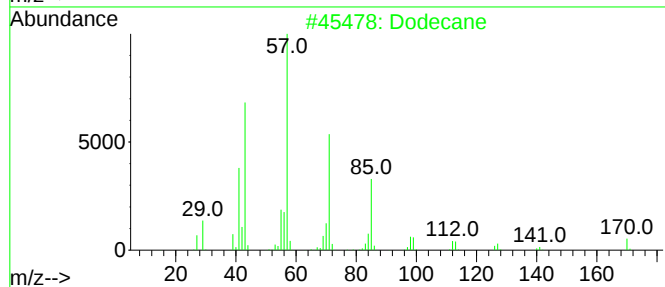
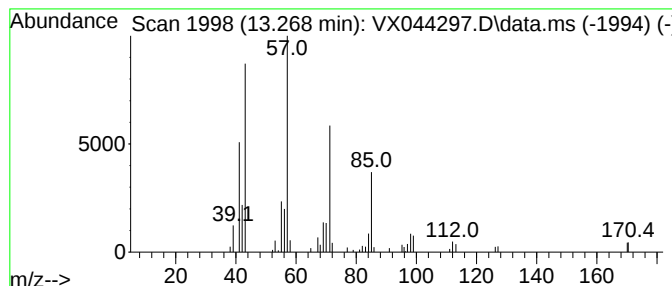
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.268	4.15 ug/L	43290	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	93
3		Dodecane	170	C12H26	000112-40-3	93
4		Dodecane	170	C12H26	000112-40-3	90
5		Tetradecane	198	C14H30	000629-59-4	86



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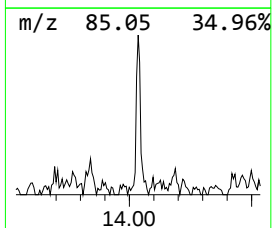
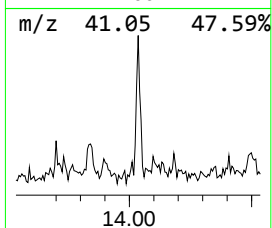
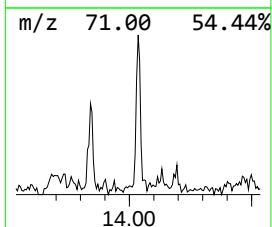
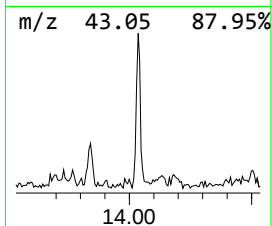
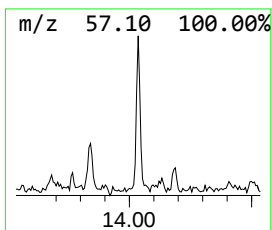
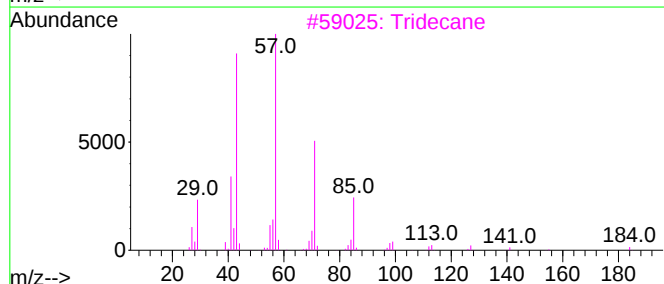
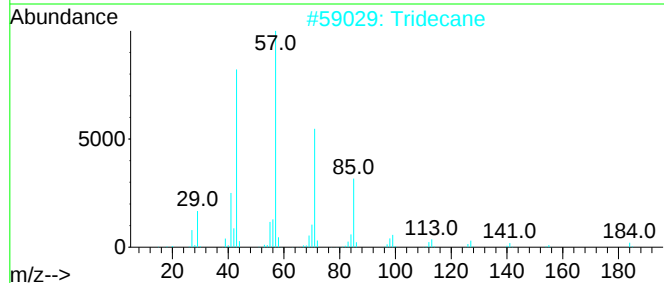
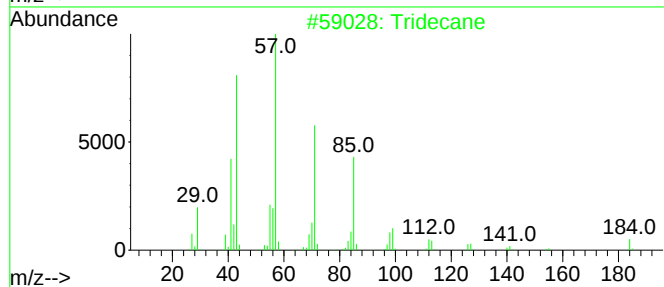
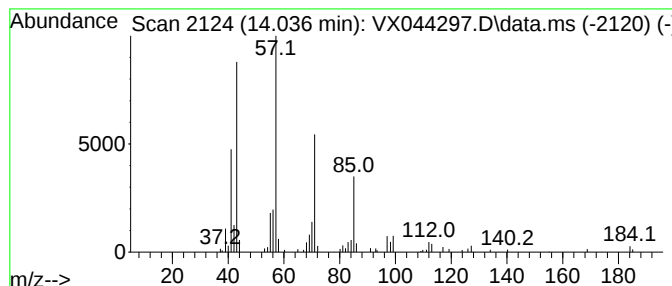
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.036	3.47 ug/L	36175	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	95
2			Tridecane	184	C13H28	000629-50-5	93
3			Tridecane	184	C13H28	000629-50-5	91
4			Tetradecane	198	C14H30	000629-59-4	91
5			1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	86



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ClientSampleId :
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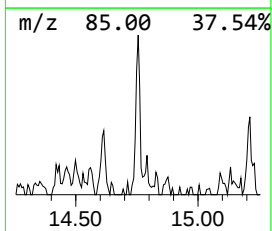
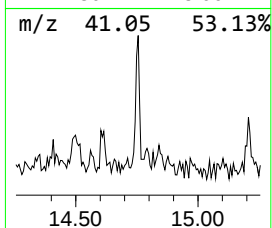
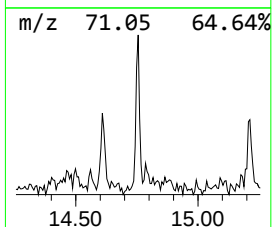
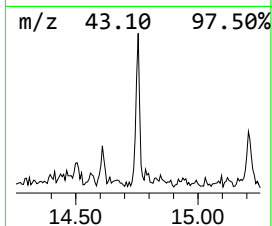
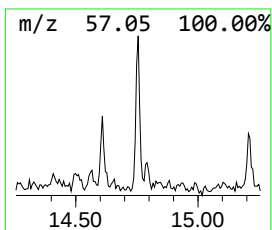
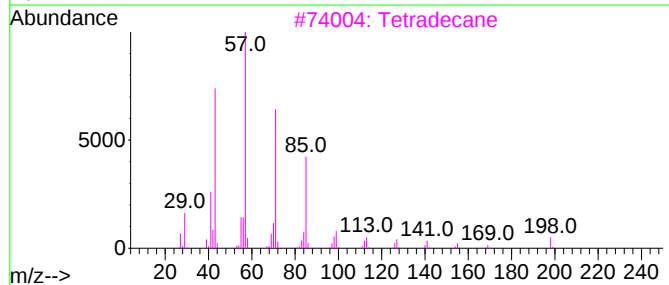
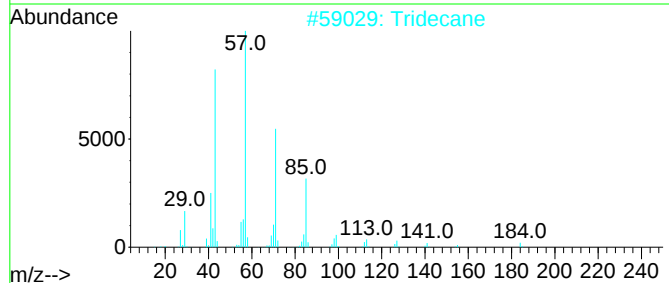
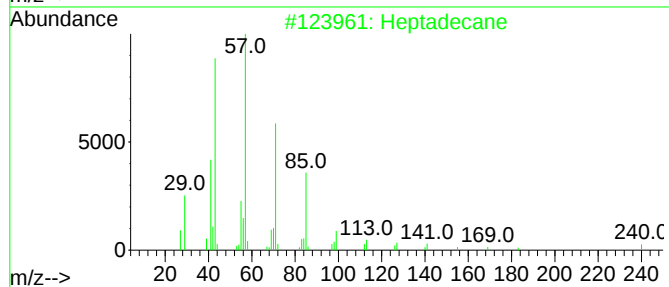
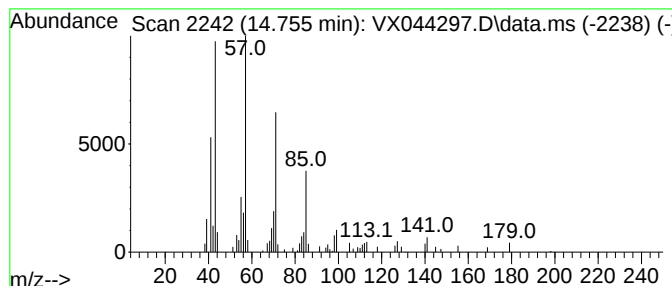
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

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.
14.755	2.65 ug/L	27580	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	86
2			Tridecane	184	C13H28	000629-50-5	86
3			Tetradecane	198	C14H30	000629-59-4	86
4			Dodecane	170	C12H26	000112-40-3	86
5			Tridecane	184	C13H28	000629-50-5	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121324\
Data File : VX044297.D
Acq On : 13 Dec 2024 21:17
Operator : JC/MD
Sample : P5153-03ME
Misc : 3.98g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E28P1ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120524WMA.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	4.2	ug/L	43290	3	12.024	521147	50.0
(DEL) Alkane: S...	14.036	3.5	ug/L	36175	3	12.024	521147	50.0
(DEL) Alkane: S...	14.755	2.6	ug/L	27580	3	12.024	521147	50.0