

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042623\
 Data File : VX035317.D
 Acq On : 26 Apr 2023 16:44
 Operator : JC/MD
 Sample : 02479-07ME
 Misc : 4.39g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EW948ME

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: VX035317.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	32	rVB2	2264	2277	0.13%	0.018%
2	1.368	42	46	66	rVB	84296	170791	9.99%	1.325%
3	1.673	84	96	100	rBV	44758	78216	4.57%	0.607%
4	2.288	191	197	211	rBV	320126	507905	29.70%	3.939%
5	2.709	261	266	272	rVV2	5166	10401	0.61%	0.081%
6	2.788	272	279	284	rVV3	3336	7353	0.43%	0.057%
7	3.428	379	384	389	rBV3	1195	2309	0.14%	0.018%
8	4.483	547	557	585	rBV	97529	357327	20.89%	2.771%
9	5.056	639	651	671	rBV	209882	653241	38.20%	5.066%
10	5.294	685	690	691	rBV2	1227	1549	0.09%	0.012%
11	5.550	724	732	739	rBV3	2063	4777	0.28%	0.037%
12	5.964	788	800	821	rBV2	594953	1710140	100.00%	13.263%
13	6.355	857	864	875	rBV5	2568	7241	0.42%	0.056%
14	6.757	921	930	946	rBV	365247	870760	50.92%	6.753%
15	7.013	968	972	977	rVB3	1061	1518	0.09%	0.012%
16	7.111	982	988	997	rBV5	5117	14884	0.87%	0.115%
17	7.208	997	1004	1011	rBV4	4224	9471	0.55%	0.073%
18	7.306	1011	1020	1037	rVV	359060	790406	46.22%	6.130%
19	7.476	1045	1048	1056	rVV6	971	1932	0.11%	0.015%
20	7.970	1119	1129	1136	rBV8	3544	10159	0.59%	0.079%
21	8.281	1175	1180	1181	rBV3	639	1094	0.06%	0.008%
22	8.324	1181	1187	1199	rBV	203731	331518	19.39%	2.571%
23	8.501	1210	1216	1224	rBV4	1178	2677	0.16%	0.021%
24	8.647	1233	1240	1257	rBV	889793	1403379	82.06%	10.884%
25	8.909	1277	1283	1284	rBV4	1492	1849	0.11%	0.014%
26	8.952	1285	1290	1304	rVV	143846	215151	12.58%	1.669%
27	9.415	1356	1366	1387	rBV	281259	760033	44.44%	5.894%
28	9.616	1395	1399	1404	rVV3	1475	2282	0.13%	0.018%
29	9.659	1404	1406	1413	rVB4	933	1593	0.09%	0.012%
30	9.909	1440	1447	1452	rVB3	1505	2434	0.14%	0.019%
31	10.013	1459	1464	1465	rBV3	1474	1786	0.10%	0.014%
32	10.055	1465	1471	1488	rVV	681762	973528	56.93%	7.550%
33	10.269	1502	1506	1508	rBV3	790	1179	0.07%	0.009%
34	10.311	1509	1513	1516	rVB4	1517	2192	0.13%	0.017%
35	10.360	1517	1521	1528	rVB2	5729	7968	0.47%	0.062%
36	10.586	1555	1558	1562	rVB4	1025	1279	0.07%	0.010%

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Integrator: RTE

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

37	10.647	1565	1568	1570	rBV3	981	1265	0.07%	0.010%
38	10.781	1583	1590	1594	rBV2	4312	5876	0.34%	0.046%
39	10.860	1599	1603	1606	rVV5	1968	3391	0.20%	0.026%
40	10.896	1606	1609	1613	rVB2	2820	3601	0.21%	0.028%
41	10.945	1613	1617	1624	rBV3	6258	9453	0.55%	0.073%
42	11.031	1628	1631	1634	rVV4	1268	1917	0.11%	0.015%
43	11.085	1634	1640	1642	rVV5	4963	8213	0.48%	0.064%
44	11.110	1642	1644	1650	rVB	4978	5213	0.30%	0.040%
45	11.201	1650	1659	1672	rBV	533146	805002	47.07%	6.243%
46	11.311	1672	1677	1685	rVB8	1293	3837	0.22%	0.030%
47	11.384	1685	1689	1693	rBV5	2576	4031	0.24%	0.031%
48	11.433	1693	1697	1699	rVV4	4144	5648	0.33%	0.044%
49	11.476	1701	1704	1710	rVB2	23842	33213	1.94%	0.258%
50	11.634	1723	1730	1734	rVB5	2954	5596	0.33%	0.043%
51	11.683	1734	1738	1740	rBV4	2708	4035	0.24%	0.031%
52	11.713	1740	1743	1747	rBV2	8903	9681	0.57%	0.075%
53	11.756	1747	1750	1759	rVB5	6210	13561	0.79%	0.105%
54	11.841	1759	1764	1766	rBV3	2001	3133	0.18%	0.024%
55	11.890	1766	1772	1776	rBV5	4101	5812	0.34%	0.045%
56	11.945	1778	1781	1783	rBV3	3769	4654	0.27%	0.036%
57	11.969	1783	1785	1789	rVB4	4169	4999	0.29%	0.039%
58	12.024	1789	1794	1800	rBV	781164	975851	57.06%	7.568%
59	12.098	1805	1806	1810	rVB2	7215	6715	0.39%	0.052%
60	12.171	1815	1818	1824	rVB4	5160	8273	0.48%	0.064%
61	12.250	1826	1831	1833	rBV6	2377	4584	0.27%	0.036%
62	12.323	1837	1843	1850	rBV	1034777	1315031	76.90%	10.198%
63	12.421	1855	1859	1864	rVB	51002	58110	3.40%	0.451%
64	12.463	1864	1866	1873	rVB5	6297	11195	0.65%	0.087%
65	12.555	1874	1881	1883	rBV6	5575	12931	0.76%	0.100%
66	12.683	1898	1902	1905	rBV3	9485	11961	0.70%	0.093%
67	12.823	1921	1925	1927	rVB4	4168	5443	0.32%	0.042%
68	12.890	1931	1936	1943	rVV6	14704	36476	2.13%	0.283%
69	12.969	1943	1949	1958	rVV6	19970	51510	3.01%	0.399%
70	13.042	1958	1961	1964	rVB4	7626	9074	0.53%	0.070%
71	13.207	1986	1988	1991	rBV4	4537	5079	0.30%	0.039%
72	13.268	1993	1998	2002	rBV	72461	95839	5.60%	0.743%
73	13.341	2008	2010	2013	rBV4	3273	3156	0.18%	0.024%
74	13.384	2013	2017	2020	rBV	23456	28579	1.67%	0.222%
75	13.500	2032	2036	2040	rBV7	4260	7790	0.46%	0.060%
76	13.701	2067	2069	2072	rBV4	6353	6349	0.37%	0.049%

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 Title : VOC Analysis

77	13.780	2078	2082	2088	rVB	23426	42168	2.47%	0.327%
78	13.841	2088	2092	2095	rBV3	13701	17370	1.02%	0.135%
79	13.987	2113	2116	2119	rBV5	4483	7581	0.44%	0.059%
80	14.036	2121	2124	2128	rVV	39075	42297	2.47%	0.328%
81	14.134	2138	2140	2143	rVB4	6655	6688	0.39%	0.052%
82	14.615	2216	2219	2220	rBV3	5619	6586	0.39%	0.051%
83	14.640	2220	2223	2226	rVB	19549	22410	1.31%	0.174%
84	14.756	2238	2242	2244	rBV2	15320	17376	1.02%	0.135%
85	14.780	2244	2246	2253	rVB	17721	23254	1.36%	0.180%
86	15.048	2287	2290	2292	rBV4	3577	5110	0.30%	0.040%
87	15.127	2299	2303	2306	rBV6	5463	7971	0.47%	0.062%
88	15.207	2314	2316	2323	rVB6	6239	9705	0.57%	0.075%
89	15.377	2341	2344	2347	rBV4	3779	4644	0.27%	0.036%
90	15.408	2347	2349	2354	rVB5	3840	5407	0.32%	0.042%
91	15.481	2356	2361	2367	rBV2	12656	23176	1.36%	0.180%
92	15.615	2378	2383	2386	rBV	13727	22911	1.34%	0.178%
93	15.694	2392	2396	2402	rVB	16145	24093	1.41%	0.187%
94	15.987	2440	2444	2454	rVB9	4662	10741	0.63%	0.083%
95	16.091	2457	2461	2467	rVB5	3415	6202	0.36%	0.048%
96	16.194	2475	2478	2482	rBV6	1587	2613	0.15%	0.020%
97	16.328	2494	2500	2511	rVB3	27030	55516	3.25%	0.431%
98	16.408	2511	2513	2516	rVB4	1346	1456	0.09%	0.011%
99	16.536	2529	2534	2535	rBV5	3074	4449	0.26%	0.035%
100	16.658	2550	2554	2555	rBV4	4350	6068	0.35%	0.047%

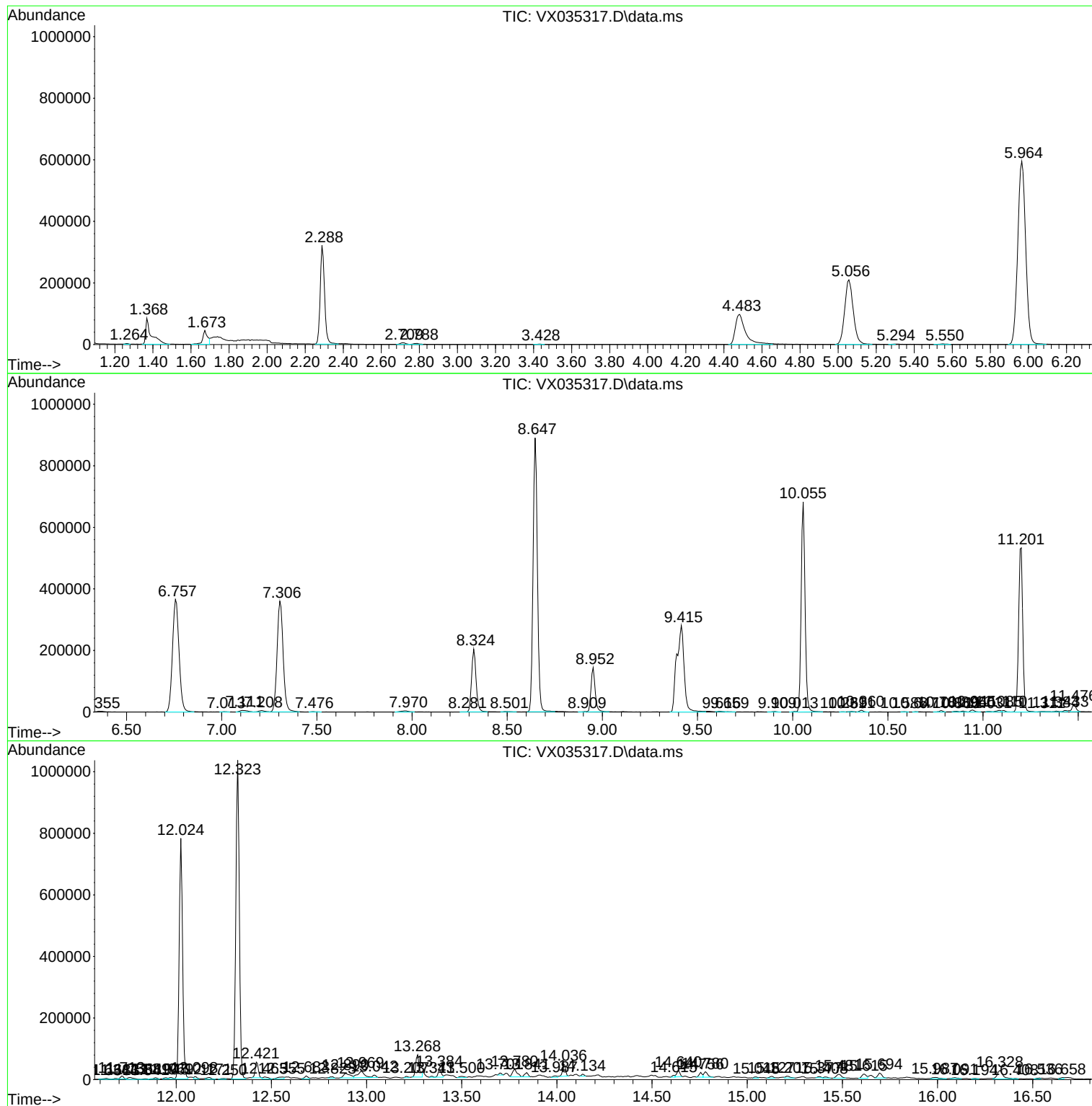
Sum of corrected areas: 12894468

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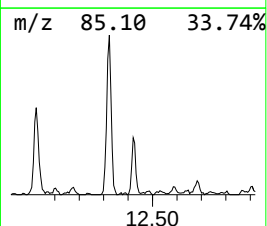
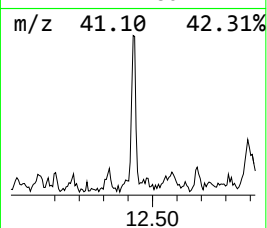
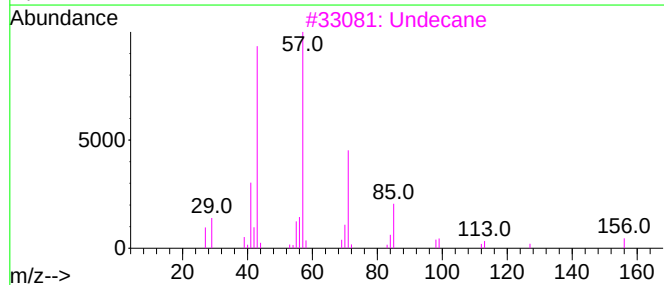
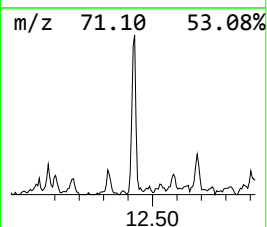
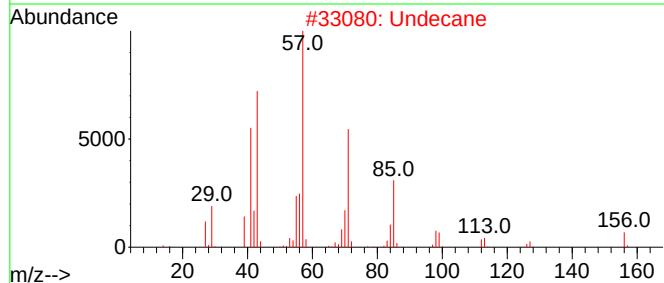
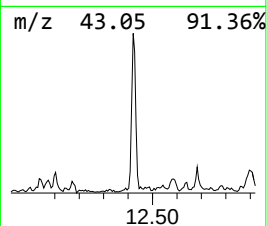
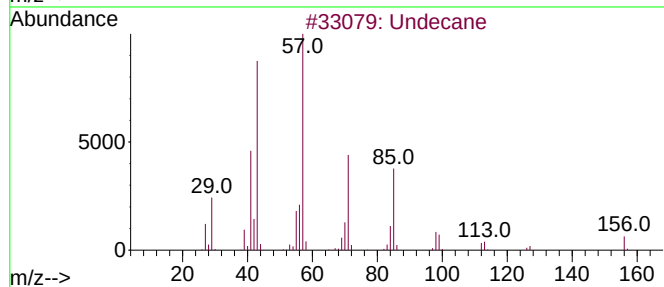
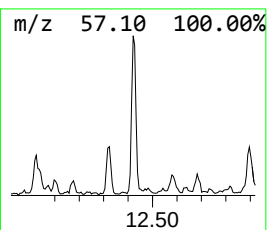
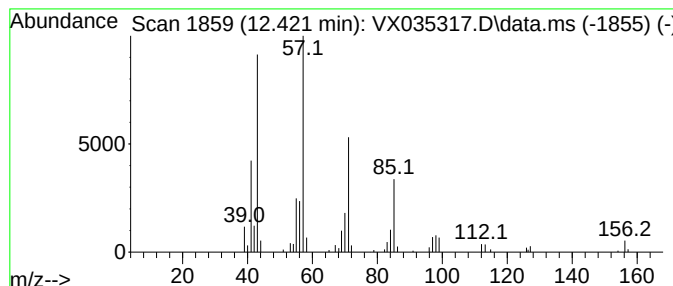
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041823WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.421	2.98 ug/L	58110	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	95
2	Undecane			156	C11H24	001120-21-4	94
3	Undecane			156	C11H24	001120-21-4	90
4	Decane			142	C10H22	000124-18-5	90
5	Carbonic acid, prop-1-en-2-yl te...			298	C18H34O3	1000382-90-9	90



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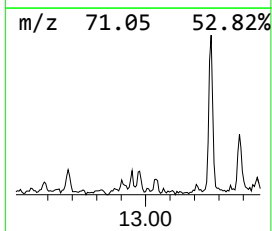
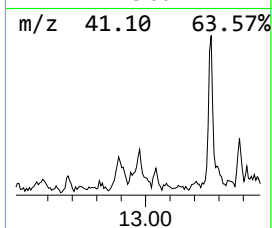
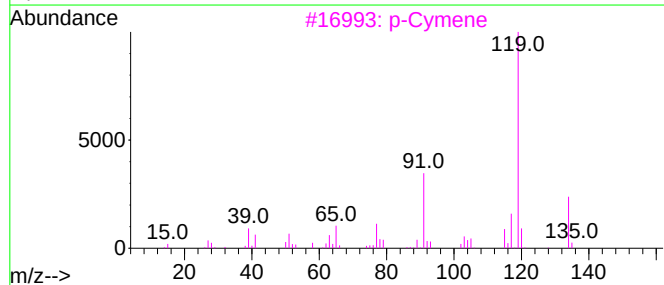
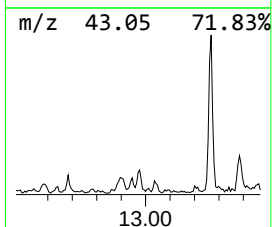
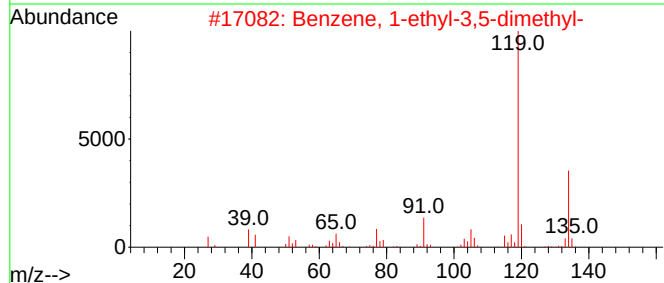
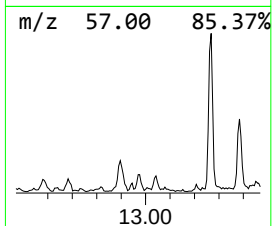
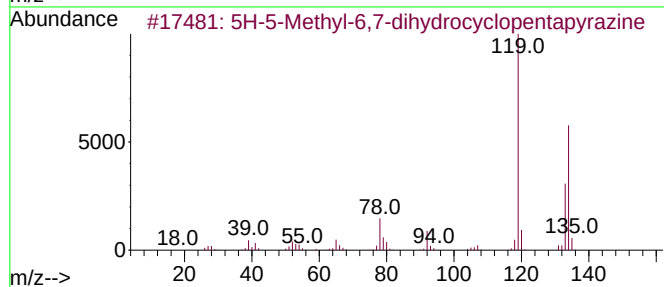
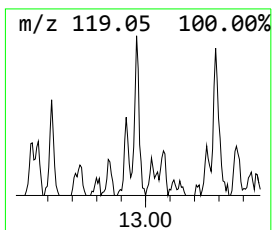
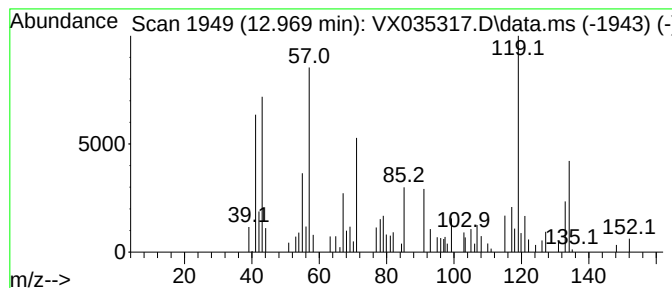
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.969	2.64 ug/L	51510	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-5-Methyl-6,7-dihydrocyclopent...	134	C8H10N2	023747-48-0	43		
2	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	38		
3	p-Cymene	134	C10H14	000099-87-6	38		
4	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	38		
5	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	38		



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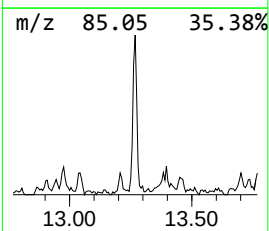
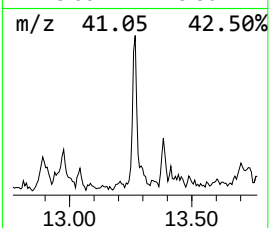
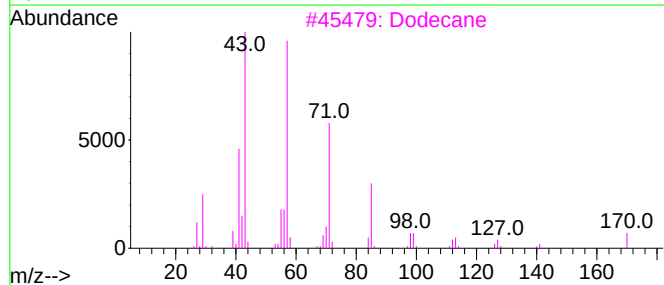
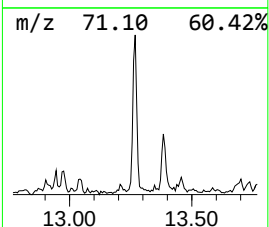
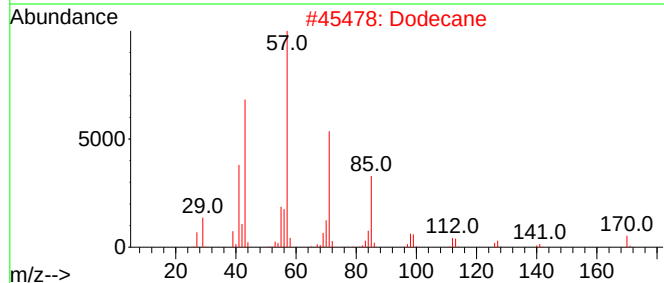
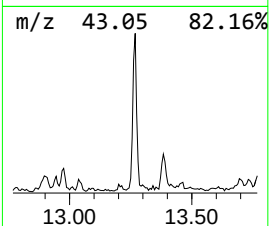
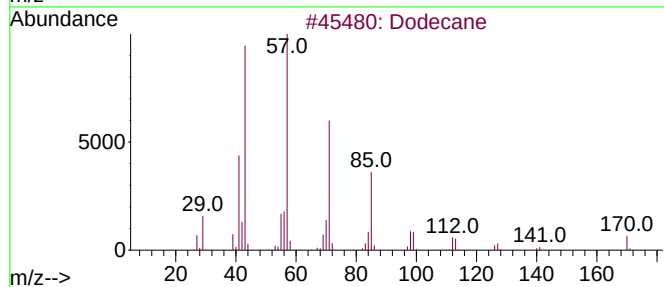
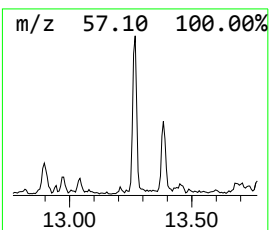
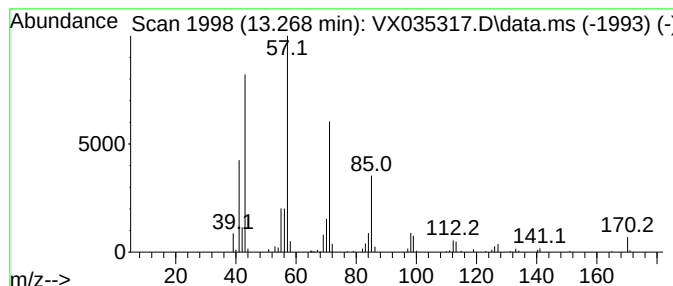
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041823WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.268	4.91 ug/L	95839	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	96
2			Dodecane	170	C12H26	000112-40-3	96
3			Dodecane	170	C12H26	000112-40-3	95
4			Dodecane	170	C12H26	000112-40-3	93
5			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042623\
Data File : VX035317.D
Acq On : 26 Apr 2023 16:44
Operator : JC/MD
Sample : 02479-07ME
Misc : 4.39g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW948ME

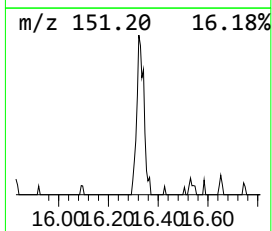
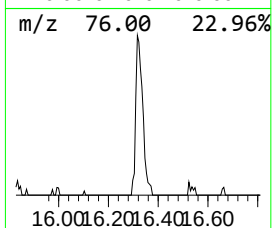
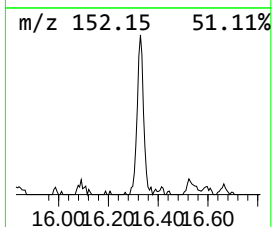
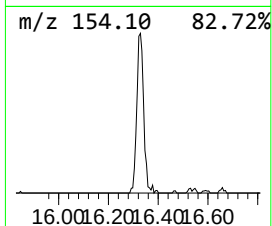
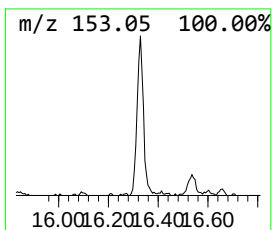
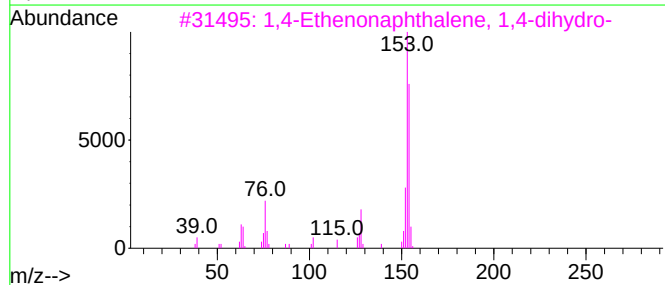
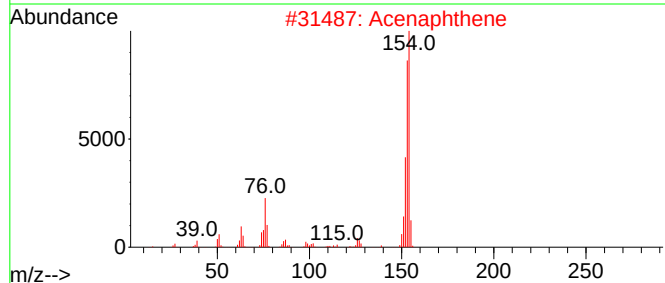
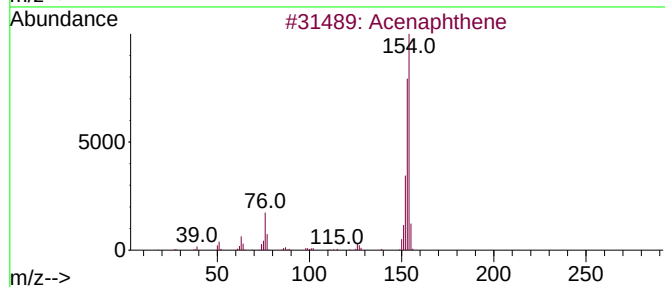
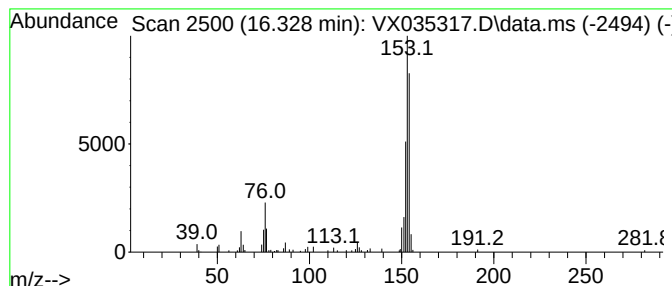
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Quant Title : VOC Analysis

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

Peak Number 5 1,4-Ethenonaphthalene, 1,4-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.328	2.84 ug/L	55516	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acenaphthene	154	C12H10	000083-32-9	74
2			Acenaphthene	154	C12H10	000083-32-9	72
3			1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	64
4			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	62
5			Acenaphthene	154	C12H10	000083-32-9	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042623\
Data File : VX035317.D
Acq On : 26 Apr 2023 16:44
Operator : JC/MD
Sample : 02479-07ME
Misc : 4.39g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW948ME

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	12.421	3.0	ug/L	58110	3	12.024	975851	50.0
unknown-01	12.969	2.6	ug/L	51510	3	12.024	975851	50.0
(DEL) Alkane: S...	13.268	4.9	ug/L	95839	3	12.024	975851	50.0
1,4-Ethenonapht...	16.328	2.8	ug/L	55516	3	12.024	975851	50.0