

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122724\
 Data File : VX044516.D
 Acq On : 27 Dec 2024 13:27
 Operator : JC/MD
 Sample : P5378-07ME
 Misc : 6.17g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 YE685ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

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: VX044516.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	26	28	31	rVB	7218	5900	0.77%	0.100%
2	1.368	43	46	61	rVB	61151	111105	14.59%	1.886%
3	1.642	89	91	95	rBV	25583	38033	4.99%	0.646%
4	2.282	190	196	205	rBV	155108	236296	31.02%	4.011%
5	2.550	239	240	243	rVB2	414	360	0.05%	0.006%
6	2.654	255	257	259	rBV3	493	350	0.05%	0.006%
7	2.788	272	279	282	rBV5	1214	2715	0.36%	0.046%
8	2.940	298	304	313	rBV4	3627	9604	1.26%	0.163%
9	3.117	327	333	334	rBV3	375	700	0.09%	0.012%
10	3.136	334	336	338	rVB2	556	442	0.06%	0.008%
11	3.264	355	357	359	rVV	523	457	0.06%	0.008%
12	3.325	363	367	369	rBV2	565	817	0.11%	0.014%
13	3.422	378	383	389	rVV5	3570	6924	0.91%	0.118%
14	3.489	393	394	397	rBV3	382	383	0.05%	0.007%
15	3.605	411	413	415	rBV3	433	421	0.06%	0.007%
16	3.727	431	433	434	rVB	537	280	0.04%	0.005%
17	3.818	445	448	450	rBV2	662	666	0.09%	0.011%
18	3.855	453	454	456	rBV	576	503	0.07%	0.009%
19	3.916	462	464	467	rBV2	432	553	0.07%	0.009%
20	4.081	489	491	492	rBV2	414	290	0.04%	0.005%
21	4.099	492	494	497	rVV2	612	643	0.08%	0.011%
22	4.123	497	498	500	rVV2	512	391	0.05%	0.007%
23	4.142	500	501	504	rVB	622	414	0.05%	0.007%
24	4.178	504	507	509	rBV2	384	476	0.06%	0.008%
25	4.245	516	518	520	rBV2	357	305	0.04%	0.005%
26	4.337	531	533	535	rBV2	369	401	0.05%	0.007%
27	4.422	545	547	548	rBV2	454	387	0.05%	0.007%
28	4.477	548	556	576	rBV	36892	148647	19.52%	2.523%
29	4.794	606	608	611	rVB3	587	514	0.07%	0.009%
30	4.824	611	613	616	rBV3	685	695	0.09%	0.012%
31	5.050	637	650	666	rBV2	100843	317531	41.69%	5.390%
32	5.251	680	683	685	rBV3	636	763	0.10%	0.013%
33	5.349	697	699	703	rBV3	458	833	0.11%	0.014%
34	5.507	723	725	726	rBV	527	335	0.04%	0.006%
35	5.525	726	728	729	rBV2	916	693	0.09%	0.012%
36	5.629	744	745	748	rBV2	484	424	0.06%	0.007%

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Instrument :
 MSVOA_X
 ClientSampleId :
 YE685ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

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	5.660	748	750	752	rVB2	493	288	0.04%	0.005%
38	5.720	758	760	761	rBV	582	478	0.06%	0.008%
39	5.824	776	777	779	rBV2	408	336	0.04%	0.006%
40	5.879	784	786	787	rBV2	518	302	0.04%	0.005%

41	5.958	787	799	814	rBV2	261572	761681	100.00%	12.930%
42	6.202	837	839	840	rBV2	431	316	0.04%	0.005%
43	6.361	860	865	869	rBV5	1286	2833	0.37%	0.048%
44	6.568	897	899	902	rVB3	421	523	0.07%	0.009%
45	6.751	920	929	943	rBV	158537	381573	50.10%	6.477%

46	7.007	969	971	972	rBV2	556	422	0.06%	0.007%
47	7.056	978	979	981	rBV2	594	612	0.08%	0.010%
48	7.123	983	990	1000	rVV9	7094	20396	2.68%	0.346%
49	7.299	1011	1019	1038	rVB	158683	350224	45.98%	5.945%
50	7.696	1082	1084	1086	rBV	648	627	0.08%	0.011%

51	7.751	1090	1093	1094	rVV4	401	375	0.05%	0.006%
52	8.043	1139	1141	1144	rBV3	508	708	0.09%	0.012%
53	8.110	1150	1152	1153	rVB	483	280	0.04%	0.005%
54	8.153	1153	1159	1160	rBV3	577	826	0.11%	0.014%
55	8.165	1160	1161	1164	rVB2	437	356	0.05%	0.006%

56	8.238	1171	1173	1174	rVV	821	510	0.07%	0.009%
57	8.275	1178	1179	1181	rVB2	433	314	0.04%	0.005%
58	8.324	1181	1187	1206	rBV	84537	149571	19.64%	2.539%
59	8.470	1209	1211	1213	rVB2	620	360	0.05%	0.006%
60	8.488	1213	1214	1217	rVB2	1008	762	0.10%	0.013%

61	8.513	1217	1218	1219	rBV	516	315	0.04%	0.005%
62	8.531	1219	1221	1223	rBV3	403	326	0.04%	0.006%
63	8.598	1230	1232	1233	rBV2	604	508	0.07%	0.009%
64	8.647	1233	1240	1250	rVV	361657	587396	77.12%	9.971%
65	8.952	1283	1290	1302	rBV	58371	96283	12.64%	1.634%

66	9.110	1313	1316	1318	rBV3	987	1112	0.15%	0.019%
67	9.171	1324	1326	1328	rVB3	610	529	0.07%	0.009%
68	9.226	1333	1335	1337	rBV3	442	496	0.07%	0.008%
69	9.263	1340	1341	1342	rBV	580	345	0.05%	0.006%
70	9.391	1357	1362	1375	rBV	183766	318823	41.86%	5.412%

71	9.701	1409	1413	1418	rBV5	1273	2390	0.31%	0.041%
72	9.823	1428	1433	1434	rBV4	956	1431	0.19%	0.024%
73	9.897	1444	1445	1448	rVB2	869	618	0.08%	0.010%
74	10.000	1460	1462	1465	rVB2	708	761	0.10%	0.013%
75	10.049	1465	1470	1484	rBV	304287	449795	59.05%	7.636%

76	10.275	1503	1507	1508	rBV3	1091	1326	0.17%	0.023%
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 ALS Vial : 9 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
 YE685ME

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

77	10.305	1509	1512	1517	rVV4	4339	7292	0.96%	0.124%
78	10.360	1517	1521	1526	rVB3	3231	4963	0.65%	0.084%
79	10.451	1531	1536	1538	rBV4	1894	2267	0.30%	0.038%
80	10.494	1541	1543	1545	rBV3	407	285	0.04%	0.005%
81	10.555	1551	1553	1554	rBV2	1140	841	0.11%	0.014%
82	10.646	1565	1568	1574	rBV5	2672	5223	0.69%	0.089%
83	10.774	1582	1589	1593	rBV4	10566	15893	2.09%	0.270%
84	10.854	1599	1602	1606	rBV4	4618	6980	0.92%	0.118%
85	10.945	1613	1617	1622	rVB5	3683	6004	0.79%	0.102%
86	11.000	1623	1626	1628	rBV4	2992	3219	0.42%	0.055%
87	11.189	1652	1657	1668	rBV	277867	401569	52.72%	6.817%
88	11.329	1677	1680	1685	rBV5	7253	13784	1.81%	0.234%
89	11.427	1693	1696	1699	rBV3	10895	16756	2.20%	0.284%
90	11.476	1701	1704	1709	rVB2	54370	68233	8.96%	1.158%
91	11.713	1740	1743	1746	rBV	36322	41950	5.51%	0.712%
92	11.939	1776	1780	1784	rBV4	25067	39602	5.20%	0.672%
93	12.018	1789	1793	1799	rBV	319766	435551	57.18%	7.394%
94	12.317	1837	1842	1848	rBV	428147	553297	72.64%	9.393%
95	12.421	1856	1859	1863	rVB	62314	66723	8.76%	1.133%
96	13.268	1995	1998	2000	rBV	29262	39609	5.20%	0.672%
97	13.774	2078	2081	2088	rVB	36807	56576	7.43%	0.960%
98	14.036	2121	2124	2128	rVB2	25967	26751	3.51%	0.454%
99	14.609	2215	2218	2220	rBV	19838	22798	2.99%	0.387%
100	14.755	2239	2242	2244	rBV	25507	27242	3.58%	0.462%

Sum of corrected areas: 5890786

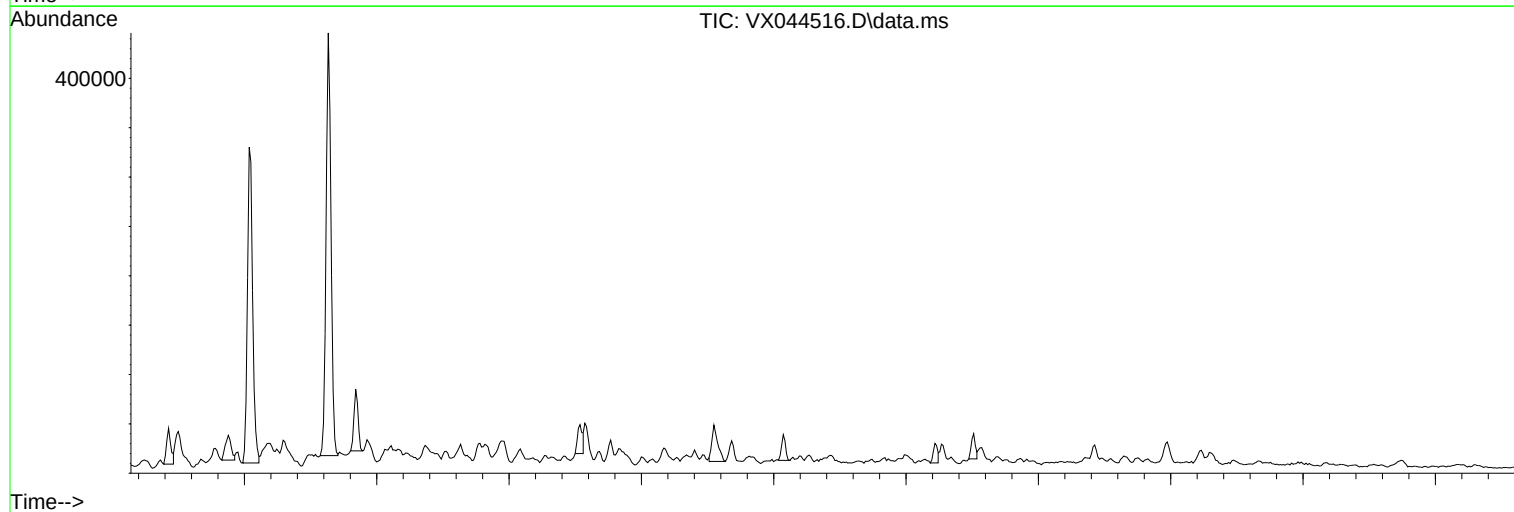
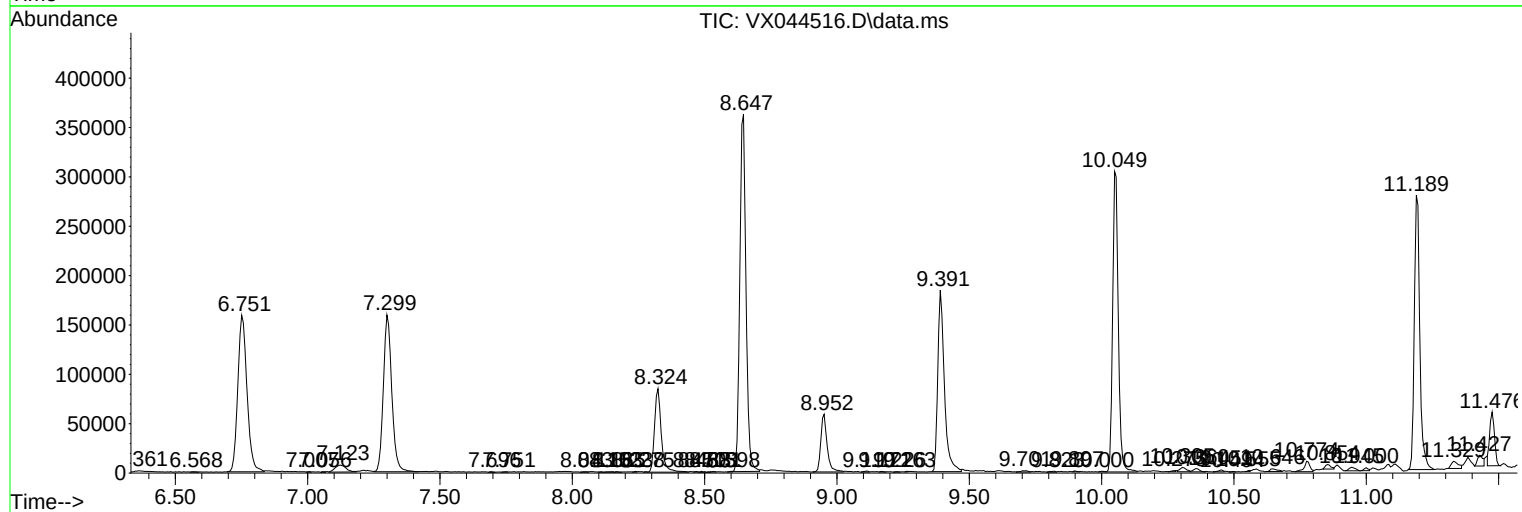
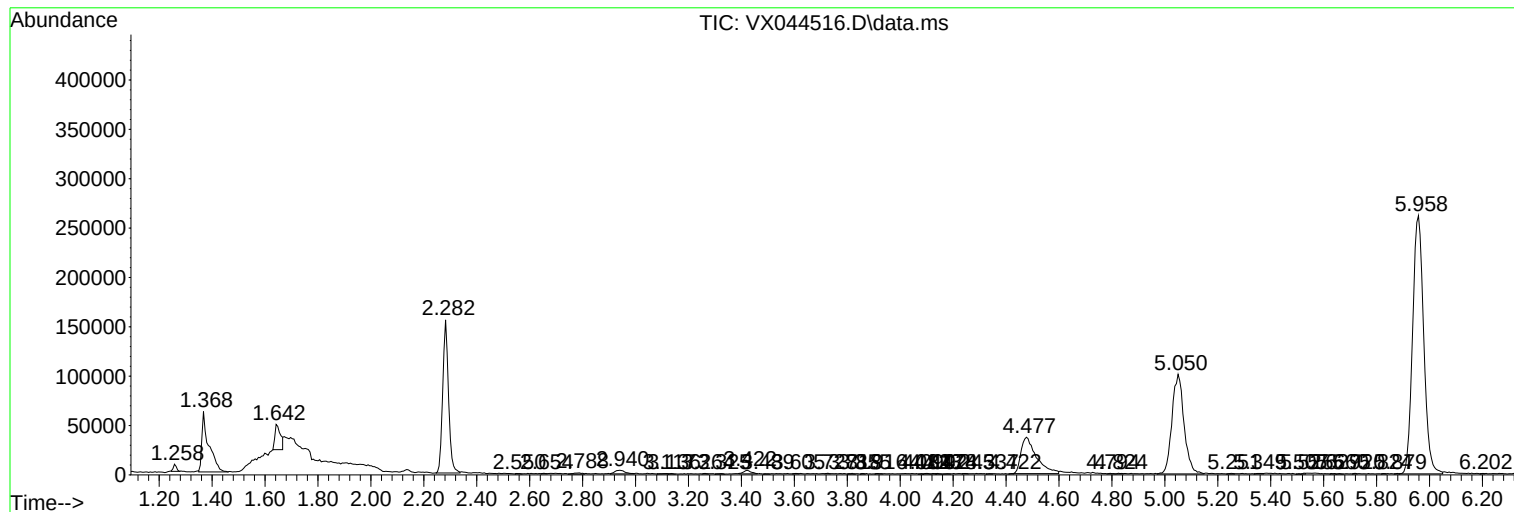
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Instrument :
MSVOA_X
ClientSampleId :
YE685ME

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



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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

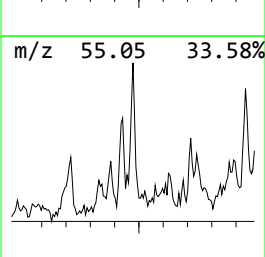
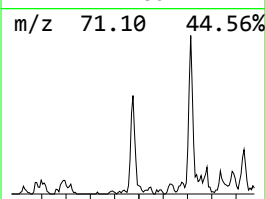
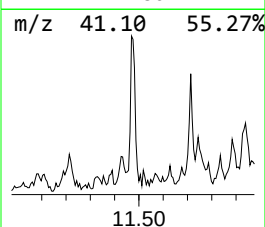
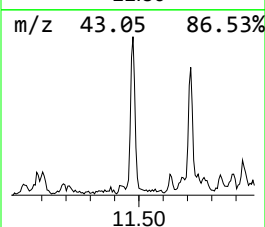
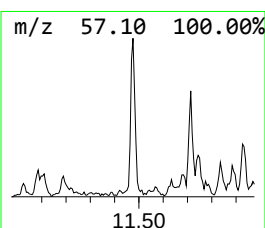
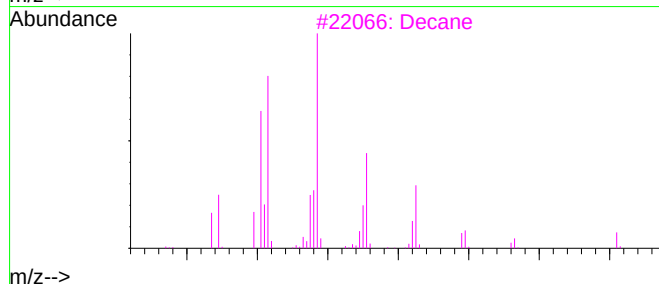
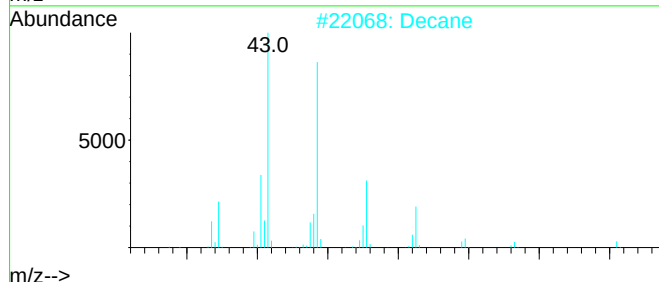
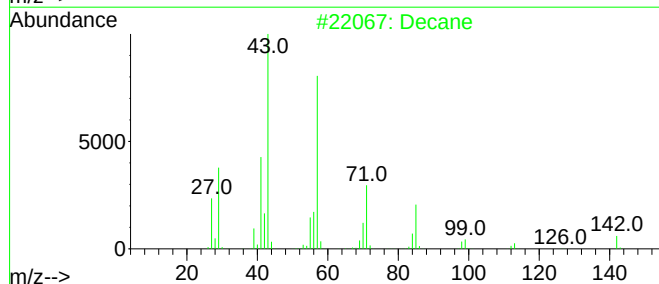
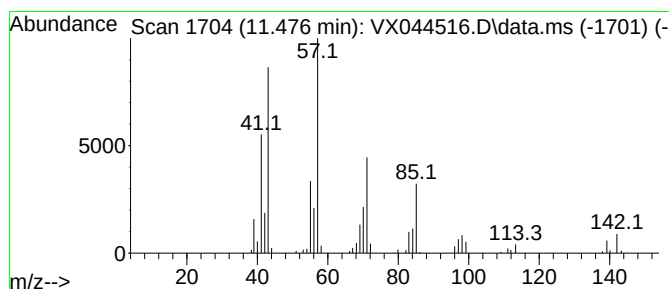
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.476	7.83 ug/L	68233	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane	142	C10H22	000124-18-5	90
2			Decane	142	C10H22	000124-18-5	83
3			Decane	142	C10H22	000124-18-5	74
4			Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	64
5			1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	59



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YE685ME

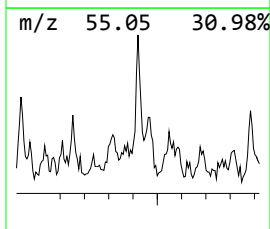
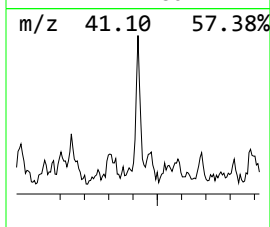
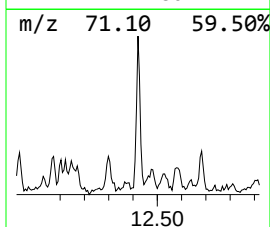
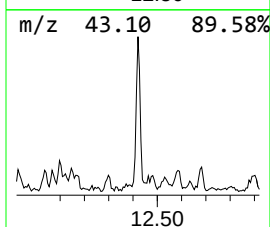
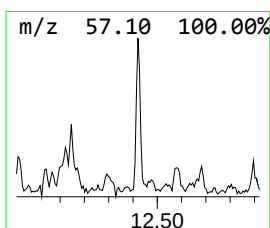
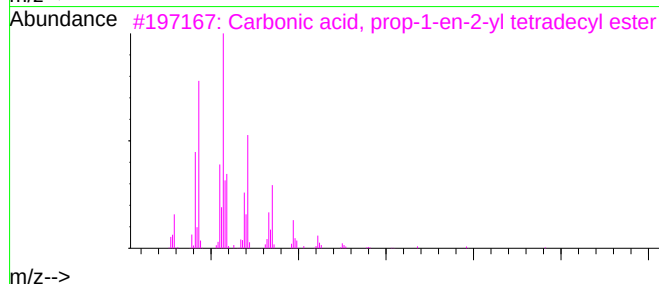
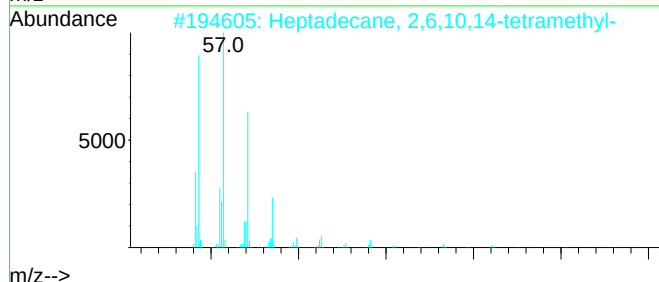
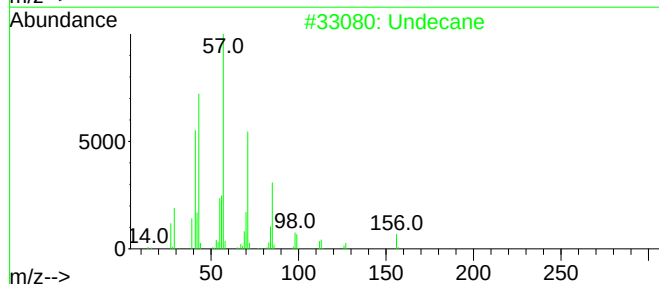
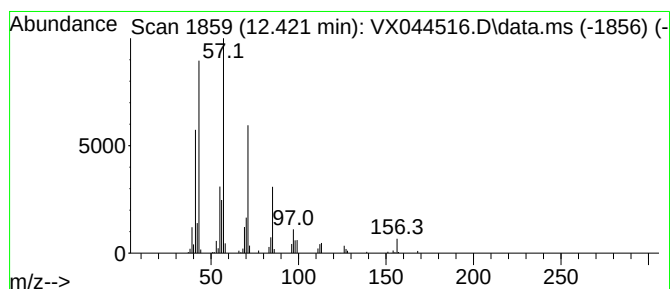
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.421	7.66 ug/L	66723	1,4-Dichlorobenzene-d4	12.018	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	93
2	Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	80
3	Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	80
4	Undecane	156	C11H24	001120-21-4	76
5	Tetradecane	198	C14H30	000629-59-4	72



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Sample : P5378-07ME
Misc : 6.17g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

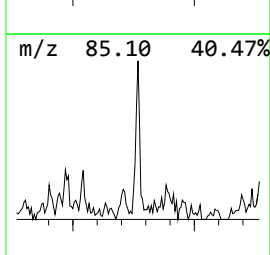
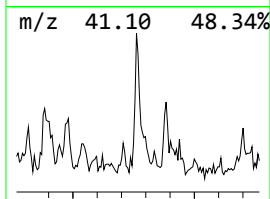
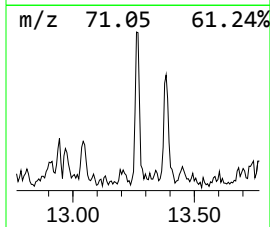
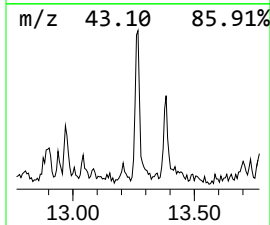
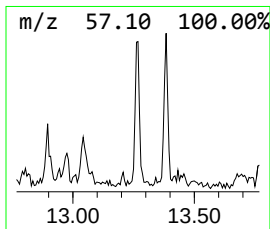
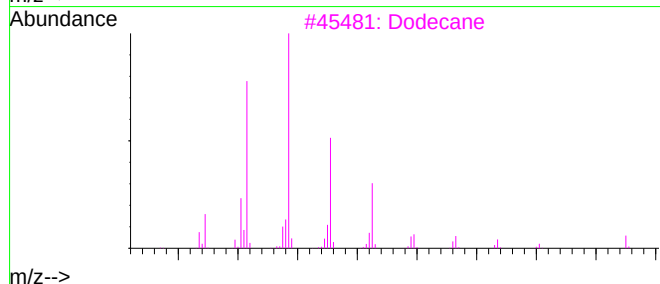
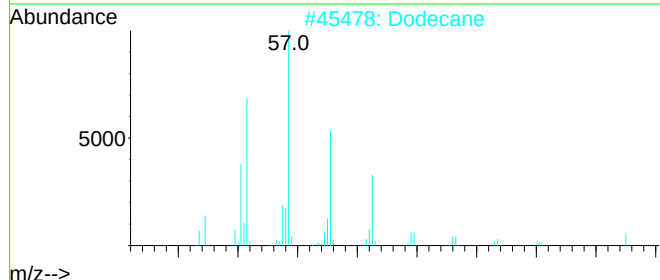
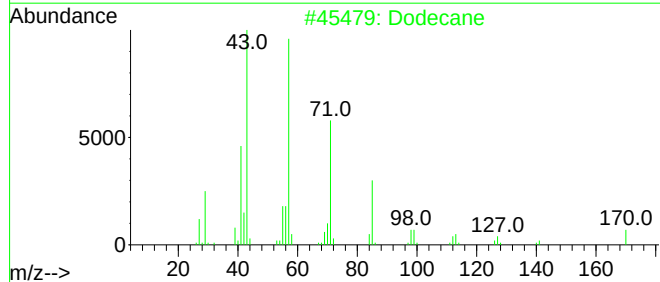
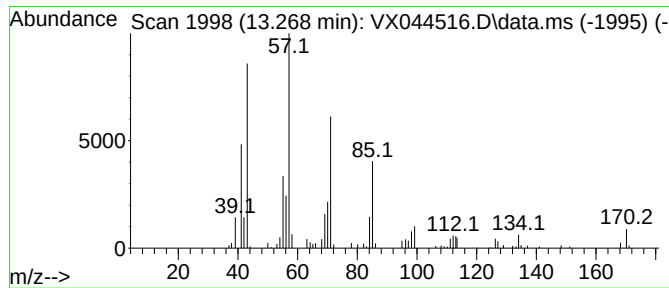
Instrument :
MSVOA_X
ClientSampleId :
YE685ME

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

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.268	4.55 ug/L	39609	1,4-Dichlorobenzene-d4		12.018	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Dodecane		170	C12H26	000112-40-3	87
2	Dodecane		170	C12H26	000112-40-3	87
3	Dodecane		170	C12H26	000112-40-3	87
4	Dodecane		170	C12H26	000112-40-3	81
5	Hexadecane		226	C16H34	000544-76-3	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122724\
Data File : VX044516.D
Acq On : 27 Dec 2024 13:27
Operator : JC/MD
Sample : P5378-07ME
Misc : 6.17g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YE685ME

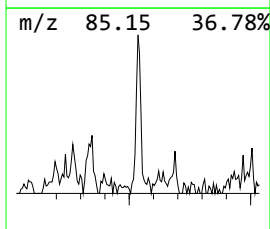
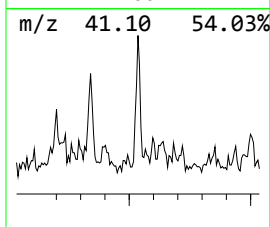
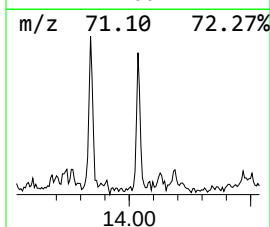
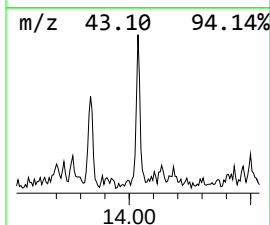
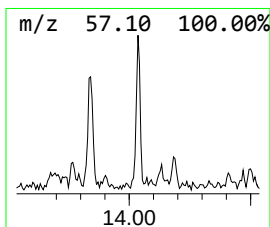
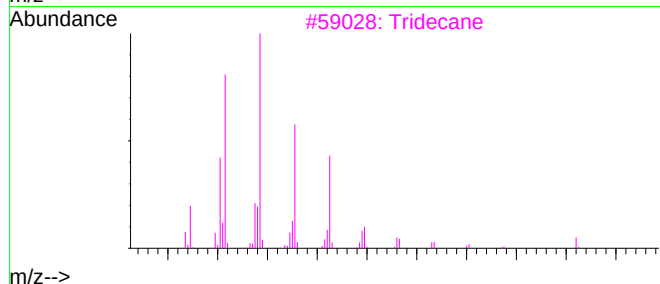
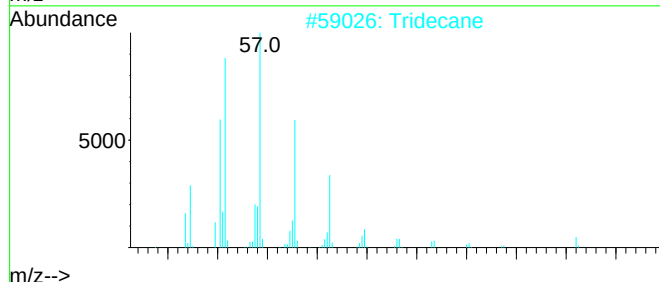
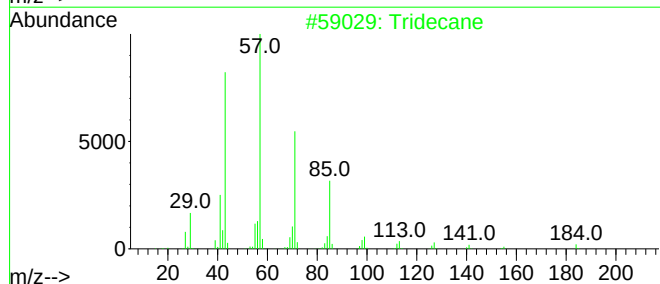
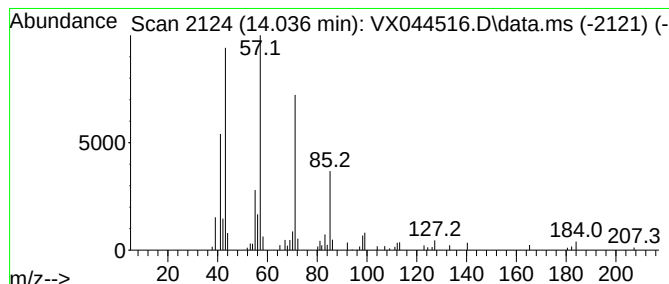
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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.036	3.07 ug/L	26751	1,4-Dichlorobenzene-d4	12.018	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	91
2	Tridecane	184	C13H28	000629-50-5	91
3	Tridecane	184	C13H28	000629-50-5	87
4	Dodecane	170	C12H26	000112-40-3	72
5	Tridecane	184	C13H28	000629-50-5	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122724\
Data File : VX044516.D
Acq On : 27 Dec 2024 13:27
Operator : JC/MD
Sample : P5378-07ME
Misc : 6.17g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YE685ME

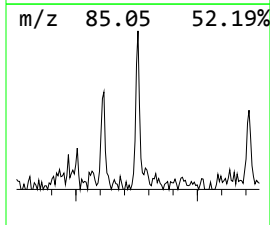
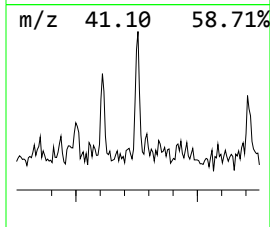
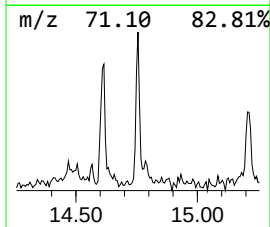
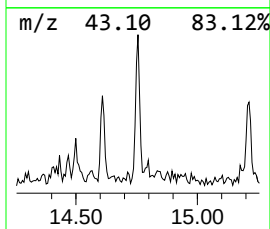
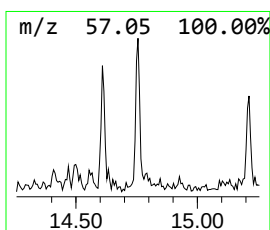
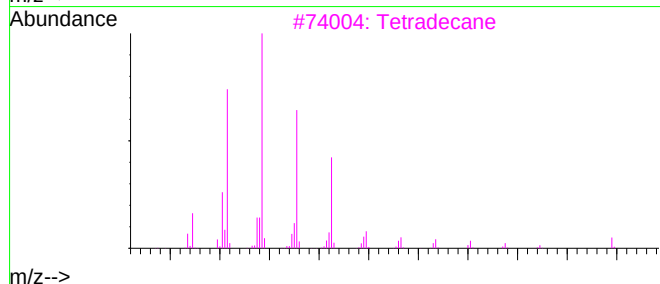
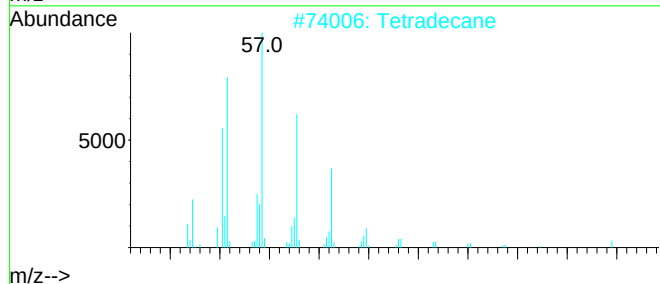
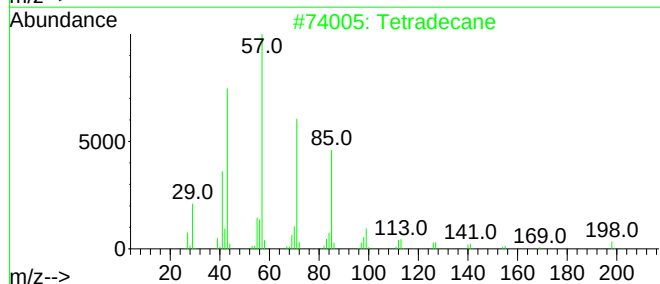
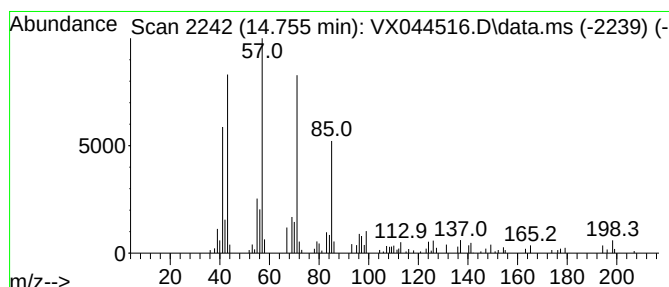
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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 10 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.755	3.13 ug/L	27242	1,4-Dichlorobenzene-d4	12.018	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	94
2	Tetradecane	198	C14H30	000629-59-4	93
3	Tetradecane	198	C14H30	000629-59-4	87
4	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	83
5	Tridecane	184	C13H28	000629-50-5	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122724\
Data File : VX044516.D
Acq On : 27 Dec 2024 13:27
Operator : JC/MD
Sample : P5378-07ME
Misc : 6.17g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YE685ME

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	11.476	7.8	ug/L	68233	3	12.018	435551	50.0
(DEL) Alkane: S...	12.421	7.7	ug/L	66723	3	12.018	435551	50.0
(DEL) Alkane: S...	13.268	4.5	ug/L	39609	3	12.018	435551	50.0
(DEL) Alkane: S...	14.036	3.1	ug/L	26751	3	12.018	435551	50.0
(DEL) Alkane: S...	14.755	3.1	ug/L	27242	3	12.018	435551	50.0