

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110921\
 Data File : VX025116.D
 Acq On : 09 Nov 2021 13:00
 Operator : JC/MD
 Sample : M4464-12ME 10X
 Misc : 7.38g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 GB7LOME

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\SFAMXLM110821WMA.M
 Title : VOC Analysis

Signal : TIC: VX025116.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	30	rVB	1478	1047	0.16%	0.015%
2	1.368	42	46	56	rVB	91464	97001	14.49%	1.384%
3	1.636	88	90	91	rBV	8772	8118	1.21%	0.116%
4	1.666	91	95	107	rVB	114578	157566	23.54%	2.248%
5	1.794	114	116	119	rBV2	1287	1267	0.19%	0.018%
6	2.306	193	200	210	rBV	150103	251497	37.57%	3.589%
7	2.386	210	213	222	rVB2	17674	31283	4.67%	0.446%
8	2.520	230	235	237	rBV2	621	1073	0.16%	0.015%
9	2.782	272	278	280	rBV5	2999	4636	0.69%	0.066%
10	2.947	300	305	307	rVV3	829	1039	0.16%	0.015%
11	3.093	324	329	338	rVV4	5105	11367	1.70%	0.162%
12	3.447	380	387	396	rVB2	10903	24228	3.62%	0.346%
13	3.611	405	414	425	rVB2	11664	29608	4.42%	0.422%
14	4.306	520	528	536	rBV8	3557	10506	1.57%	0.150%
15	4.489	544	558	570	rBV2	212401	653487	97.62%	9.325%
16	5.062	641	652	669	rVV2	95982	284990	42.57%	4.067%
17	5.385	701	705	707	rBV4	912	1190	0.18%	0.017%
18	5.483	717	721	722	rBV3	1356	1905	0.28%	0.027%
19	5.818	773	776	777	rBV2	1523	1975	0.30%	0.028%
20	5.970	790	801	816	rVV3	225166	669401	100.00%	9.552%
21	6.239	843	845	847	rBV2	1466	1588	0.24%	0.023%
22	6.342	858	862	865	rBV4	745	1313	0.20%	0.019%
23	6.611	895	906	913	rBV7	3075	8458	1.26%	0.121%
24	6.763	922	931	942	rBV	160978	386267	57.70%	5.512%
25	6.982	964	967	971	rVV2	630	997	0.15%	0.014%
26	7.123	979	990	998	rVB6	5791	16296	2.43%	0.233%
27	7.312	1012	1021	1030	rBV	144654	316034	47.21%	4.510%
28	7.495	1044	1051	1056	rVV5	1494	3147	0.47%	0.045%
29	7.775	1094	1097	1100	rBV3	704	889	0.13%	0.013%
30	7.806	1100	1102	1104	rVV3	836	810	0.12%	0.012%
31	7.958	1124	1127	1129	rBV2	1064	1215	0.18%	0.017%
32	7.982	1129	1131	1135	rVV2	1694	2154	0.32%	0.031%
33	8.104	1146	1151	1156	rBV4	1778	2874	0.43%	0.041%
34	8.275	1174	1179	1182	rBV	1869	3208	0.48%	0.046%
35	8.324	1182	1187	1201	rVB	91154	154009	23.01%	2.198%
36	8.440	1201	1206	1208	rBV4	1488	2496	0.37%	0.036%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM110821WMA.M
 Title : VOC Analysis

37	8.586	1223	1230	1234	rBV4	5058	11359	1.70%	0.162%
38	8.653	1234	1241	1247	rVV	327477	522399	78.04%	7.454%
39	8.720	1247	1252	1264	rVB	408285	629076	93.98%	8.977%
40	8.915	1280	1284	1285	rBV3	2886	3885	0.58%	0.055%
41	8.952	1285	1290	1300	rVB	72639	109867	16.41%	1.568%
42	9.098	1311	1314	1318	rVB2	709	1002	0.15%	0.014%
43	9.391	1356	1362	1375	rVV	222701	328098	49.01%	4.682%
44	9.561	1387	1390	1394	rVB5	2149	3034	0.45%	0.043%
45	9.622	1397	1400	1403	rVB2	2042	2844	0.42%	0.041%
46	9.830	1428	1434	1436	rBV3	1844	3051	0.46%	0.044%
47	9.909	1443	1447	1451	rVB4	3380	4755	0.71%	0.068%
48	10.012	1459	1464	1466	rBV4	3417	5538	0.83%	0.079%
49	10.055	1466	1471	1481	rVB	344933	460319	68.77%	6.569%
50	10.195	1489	1494	1498	rVB5	1559	2225	0.33%	0.032%
51	10.268	1503	1506	1508	rBV2	2032	2295	0.34%	0.033%
52	10.360	1517	1521	1530	rVB2	21998	31412	4.69%	0.448%
53	10.451	1533	1536	1543	rVB4	1413	2449	0.37%	0.035%
54	10.531	1546	1549	1551	rBV2	932	1307	0.20%	0.019%
55	10.592	1552	1559	1562	rBV5	7445	10603	1.58%	0.151%
56	10.677	1566	1573	1576	rBV6	3599	7751	1.16%	0.111%
57	10.787	1583	1591	1596	rBV3	18013	29628	4.43%	0.423%
58	10.860	1599	1603	1606	rVV3	12997	19711	2.94%	0.281%
59	10.896	1606	1609	1614	rVB4	11467	16062	2.40%	0.229%
60	10.951	1614	1618	1623	rVB5	2944	4871	0.73%	0.070%
61	11.000	1623	1626	1628	rBV3	3710	4503	0.67%	0.064%
62	11.085	1637	1640	1642	rBV4	11365	11996	1.79%	0.171%
63	11.195	1651	1658	1671	rBV	244399	337244	50.38%	4.812%
64	11.311	1674	1677	1679	rBV2	3032	3452	0.52%	0.049%
65	11.396	1686	1691	1693	rBV5	5847	9837	1.47%	0.140%
66	11.439	1693	1698	1700	rVV3	10650	17901	2.67%	0.255%
67	11.482	1701	1705	1710	rVB	95360	113429	16.94%	1.619%
68	11.689	1735	1739	1740	rBV3	4582	5965	0.89%	0.085%
69	11.719	1740	1744	1747	rVV	21988	27094	4.05%	0.387%
70	11.756	1747	1750	1753	rVB3	10753	14306	2.14%	0.204%
71	11.841	1760	1764	1767	rBV5	4160	6803	1.02%	0.097%
72	11.945	1778	1781	1784	rBV3	8653	12064	1.80%	0.172%
73	12.024	1789	1794	1800	rBV	336251	419954	62.74%	5.993%
74	12.079	1800	1803	1805	rVV4	6892	7620	1.14%	0.109%
75	12.104	1805	1807	1810	rVB2	8713	9148	1.37%	0.131%
76	12.268	1827	1834	1837	rBV2	9331	16508	2.47%	0.236%

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 Title : VOC Analysis

77	12.323	1838	1843	1850	rVB	342954	442947	66.17%	6.321%
78	12.427	1856	1860	1864	rVB2	62943	68411	10.22%	0.976%
79	12.561	1875	1882	1884	rBV7	6214	15145	2.26%	0.216%
80	12.689	1899	1903	1906	rVB5	3568	4720	0.71%	0.067%
81	12.799	1918	1921	1922	rBV2	2056	2326	0.35%	0.033%
82	12.896	1933	1937	1939	rBV4	3934	6801	1.02%	0.097%
83	13.213	1987	1989	1992	rBV4	1435	1316	0.20%	0.019%
84	13.268	1994	1998	2007	rVB3	20389	31466	4.70%	0.449%
85	13.384	2014	2017	2021	rBV2	5905	7526	1.12%	0.107%
86	13.591	2047	2051	2053	rBV4	941	1393	0.21%	0.020%
87	13.701	2064	2069	2072	rBV6	2115	3617	0.54%	0.052%
88	13.847	2089	2093	2096	rVB2	4480	6263	0.94%	0.089%
89	14.042	2120	2125	2129	rBV2	14678	16541	2.47%	0.236%
90	14.073	2129	2130	2131	rBV	1240	792	0.12%	0.011%
91	14.408	2182	2185	2187	rBV2	1120	1353	0.20%	0.019%
92	14.499	2197	2200	2202	rBV3	1444	1652	0.25%	0.024%
93	14.615	2216	2219	2223	rBV3	2852	3855	0.58%	0.055%
94	14.762	2237	2243	2246	rBV	5874	8268	1.24%	0.118%
95	14.981	2277	2279	2284	rVB2	661	810	0.12%	0.012%
96	15.194	2310	2314	2315	rBV2	918	1026	0.15%	0.015%
97	15.493	2359	2363	2367	rBV4	1866	2476	0.37%	0.035%
98	15.828	2415	2418	2420	rBV2	945	834	0.12%	0.012%
99	16.353	2501	2504	2505	rBV2	656	813	0.12%	0.012%
100	16.371	2505	2507	2511	rVV4	859	1208	0.18%	0.017%

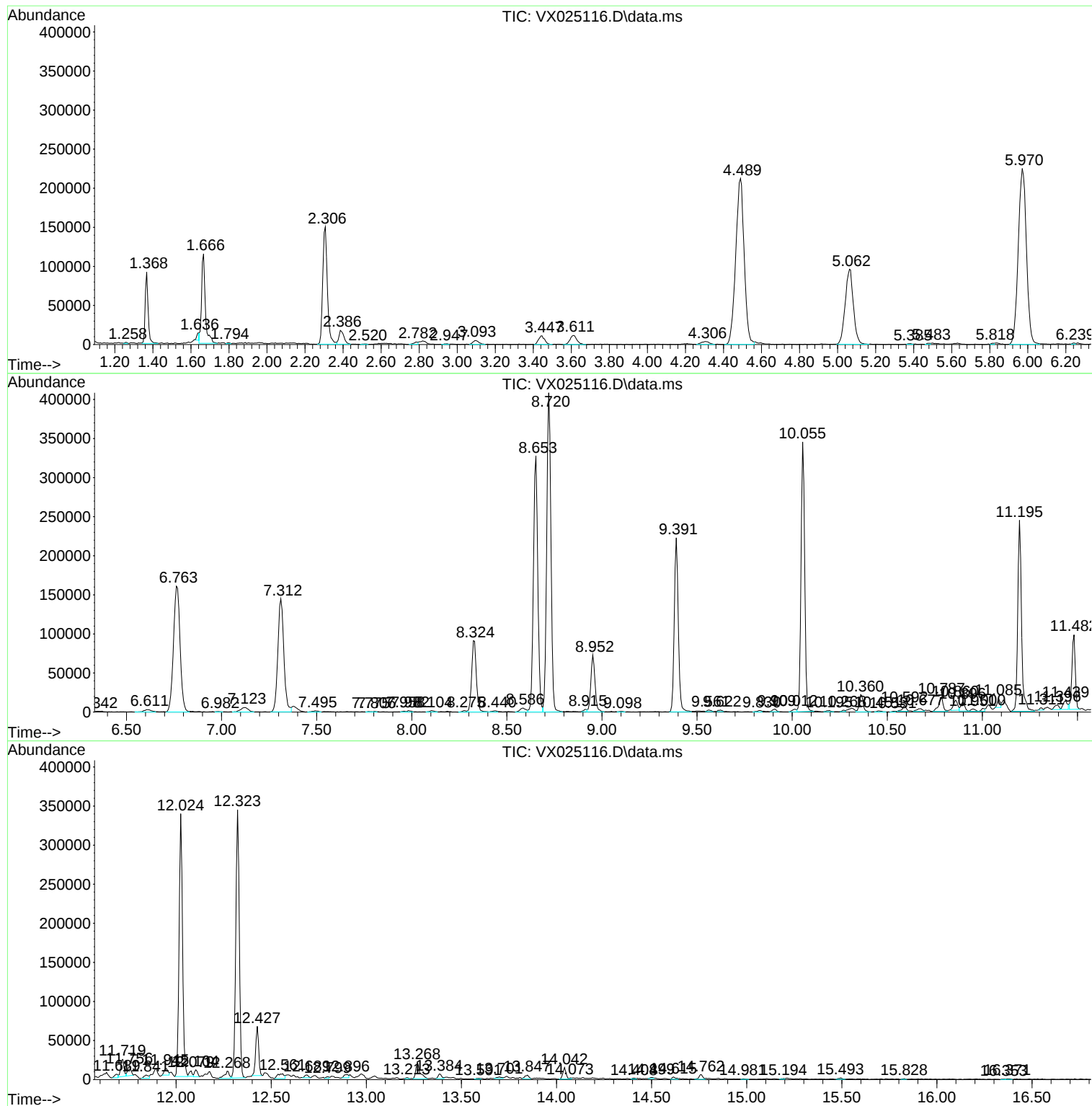
Sum of corrected areas: 7007863

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Instrument :
MSVOA_X
ClientSampleId :
GB7LOME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML110821WMA.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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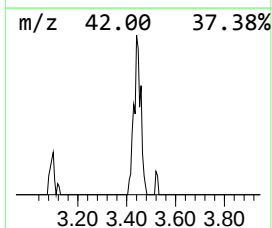
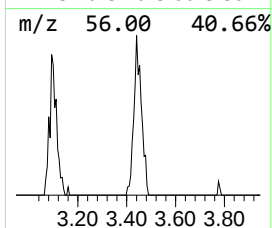
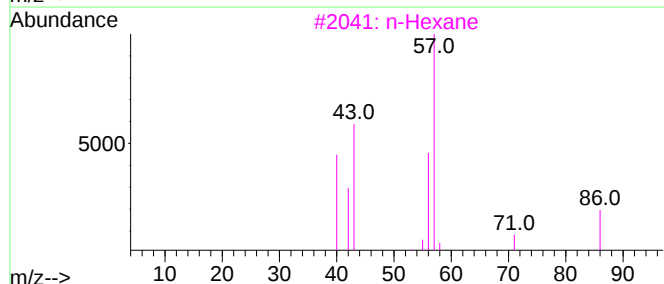
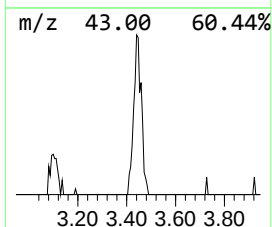
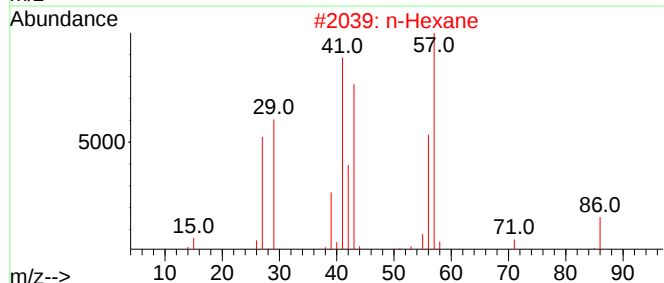
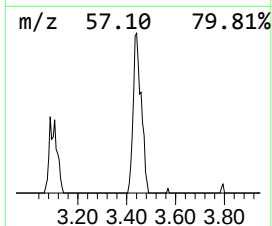
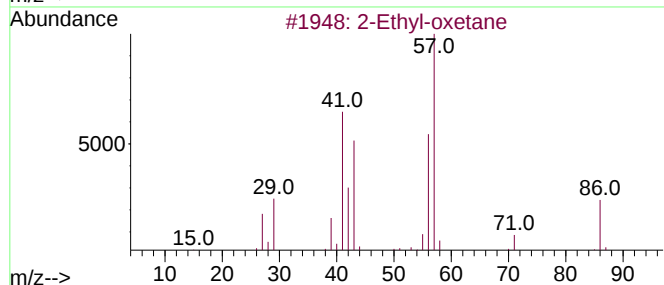
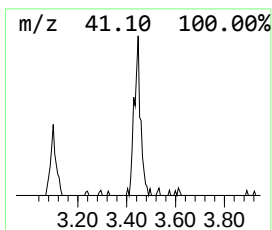
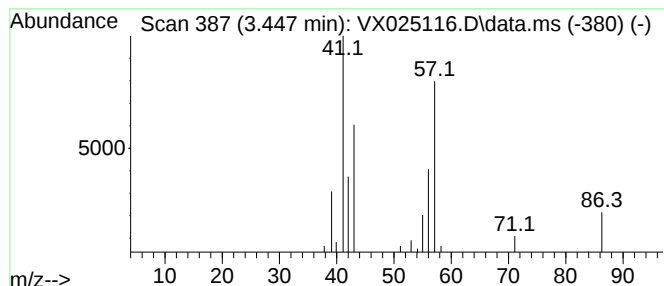
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM110821WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 2-Ethyl-oxetane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.447	3.14 ug/L	24228	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	72
2			n-Hexane	86	C6H14	000110-54-3	50
3			n-Hexane	86	C6H14	000110-54-3	45
4			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	40
5			1-Propene, 2-methyl-	56	C4H8	000115-11-7	38



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GB7L0ME

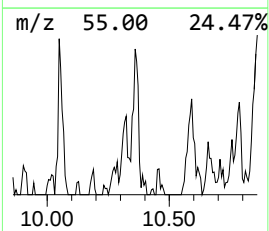
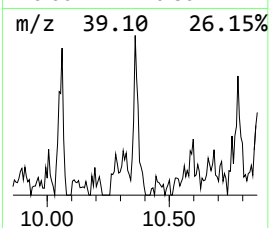
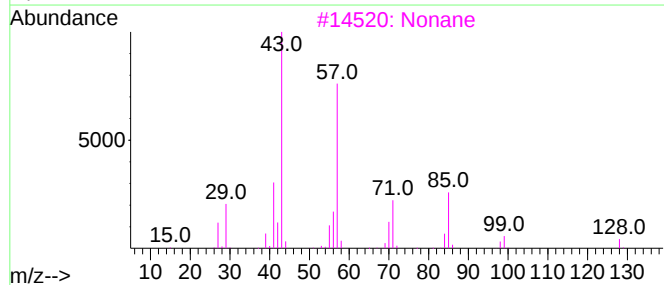
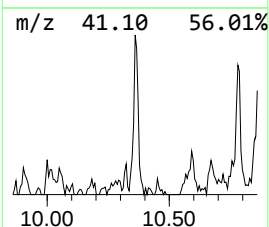
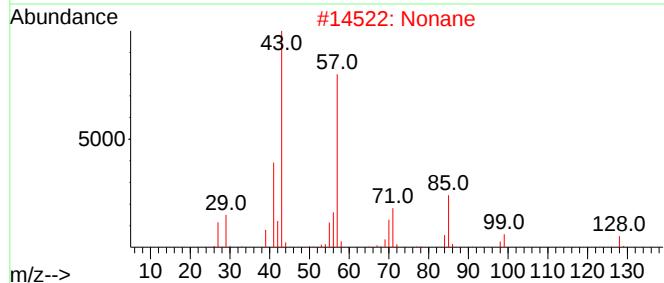
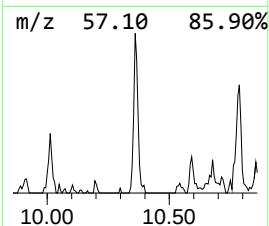
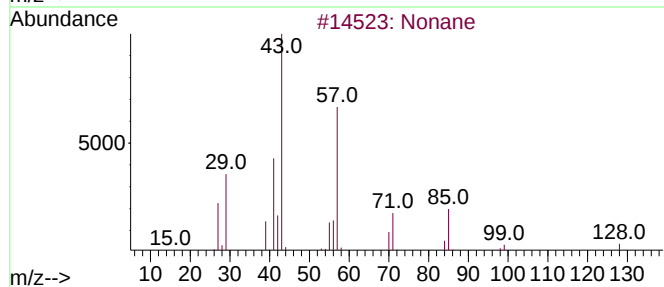
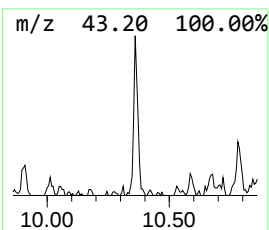
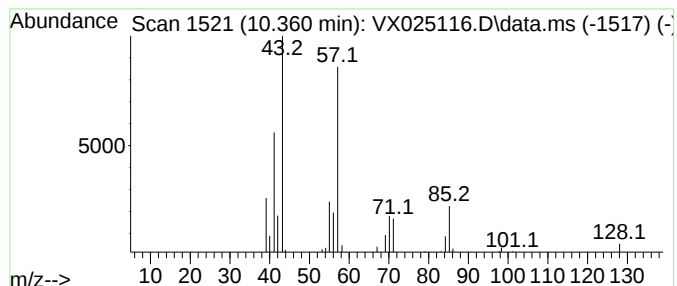
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM110821WMA.M
Quant Title : VOC Analysis

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.
10.360	3.41 ug/L	31412	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane	128	C9H20	000111-84-2	90
2			Nonane	128	C9H20	000111-84-2	86
3			Nonane	128	C9H20	000111-84-2	72
4			Nonane	128	C9H20	000111-84-2	72
5			Undecane, 5,7-dimethyl-	184	C13H28	017312-83-3	64



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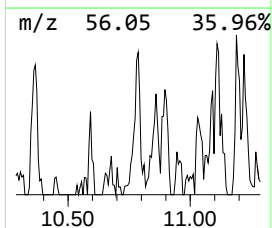
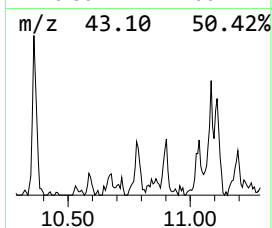
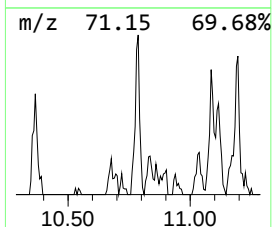
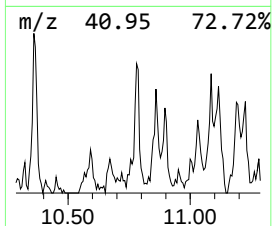
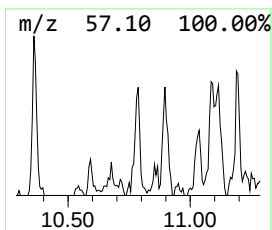
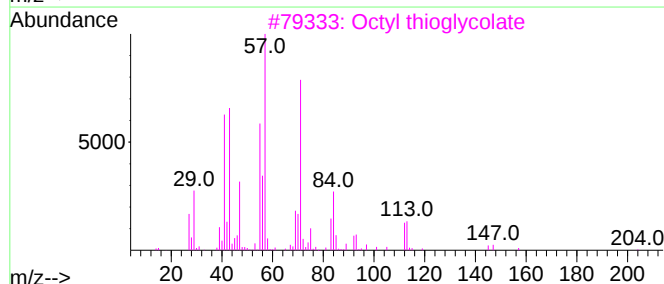
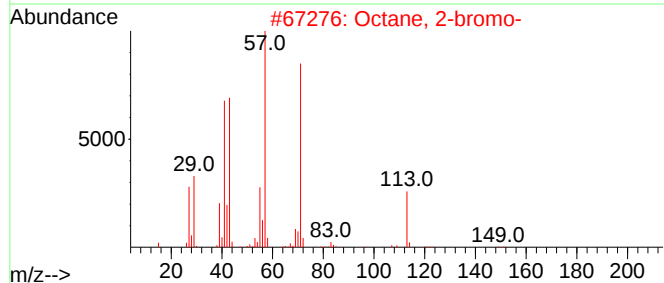
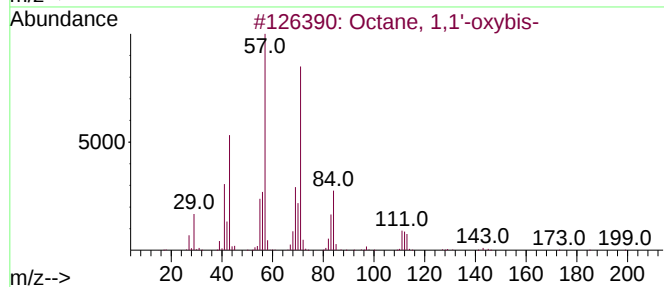
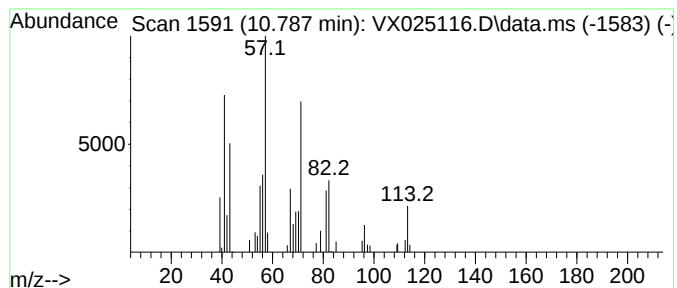
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML110821WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.787	3.22 ug/L	29628	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 1,1'-oxybis-			242	C16H34O	000629-82-3	47
2	Octane, 2-bromo-			192	C8H17Br	000557-35-7	43
3	Octyl thioglycolate			204	C10H20O2S	007664-80-4	43
4	2-Nonen-1-ol			142	C9H18O	022104-79-6	43
5	Octane, 3,6-dimethyl-			142	C10H22	015869-94-0	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110921\
Data File : VX025116.D
Acq On : 09 Nov 2021 13:00
Operator : JC/MD
Sample : M4464-12ME 10X
Misc : 7.38g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

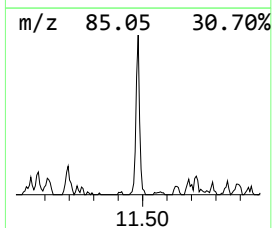
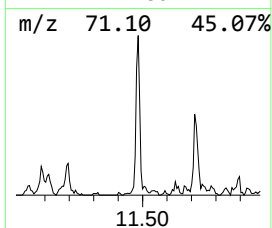
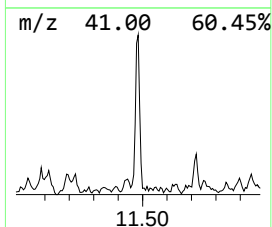
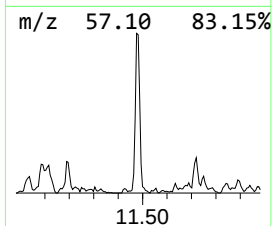
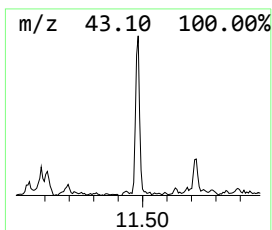
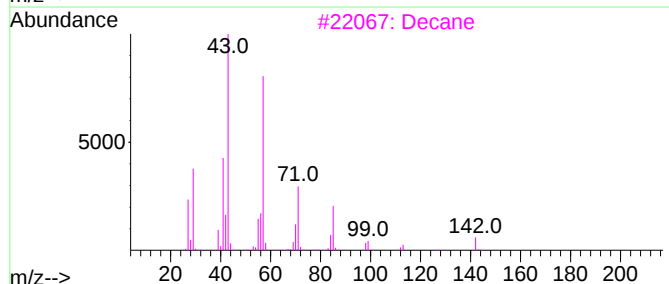
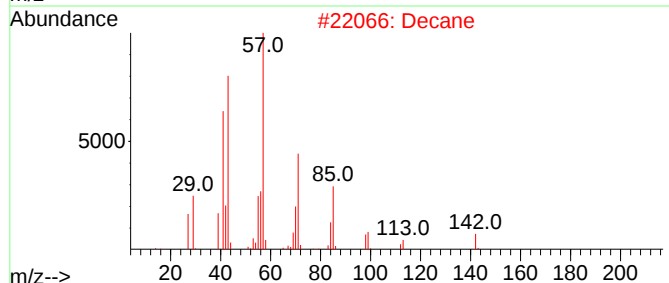
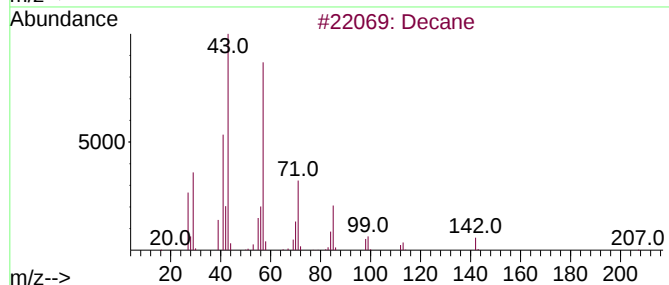
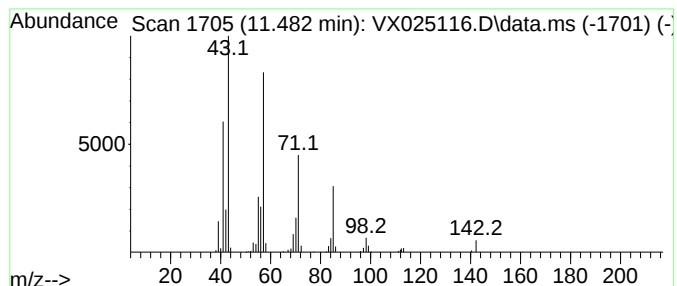
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM110821WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
11.482	13.50 ug/L	113429	1,4-Dichlorobenzene-d4			12.024
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Decane	142	C10H22	000124-18-5	91
2		Decane	142	C10H22	000124-18-5	87
3		Decane	142	C10H22	000124-18-5	80
4		Nonane	128	C9H20	000111-84-2	64
5		Tetradecane	198	C14H30	000629-59-4	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110921\
Data File : VX025116.D
Acq On : 09 Nov 2021 13:00
Operator : JC/MD
Sample : M4464-12ME 10X
Misc : 7.38g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GB7LOME

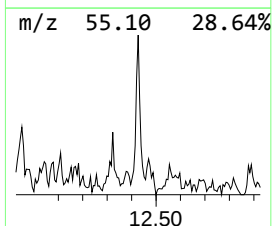
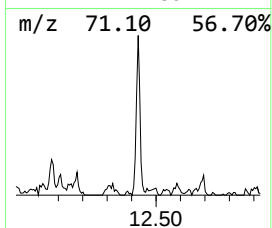
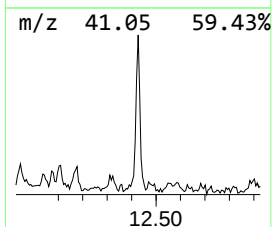
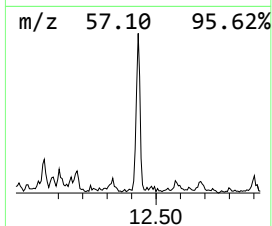
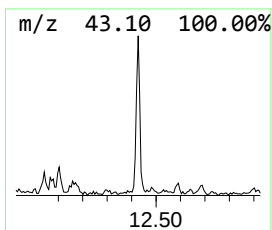
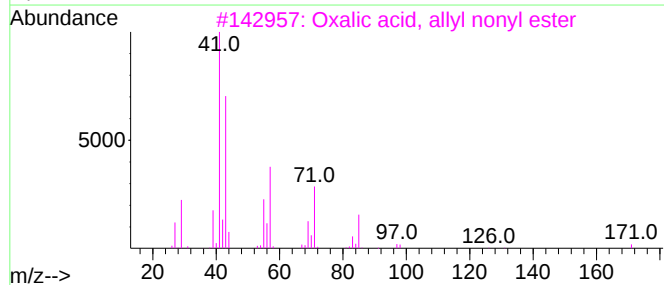
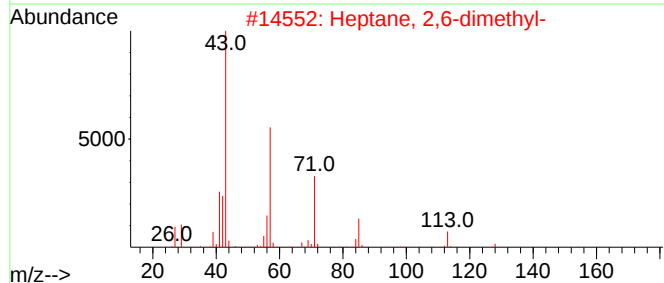
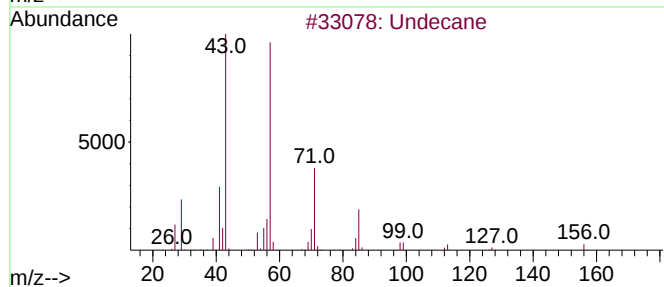
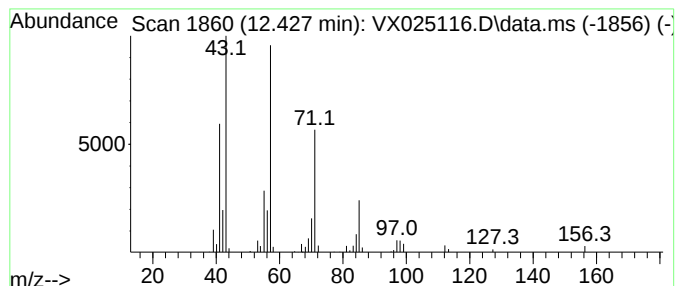
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Quant Title : VOC Analysis

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.427	8.15 ug/L	68411	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane	156	C11H24	001120-21-4	87
2			Heptane, 2,6-dimethyl-	128	C9H20	001072-05-5	80
3			Oxalic acid, allyl nonyl ester	256	C14H24O4	1000309-23-7	72
4			Undecane	156	C11H24	001120-21-4	53
5			Octane, 2,7-dimethyl-	142	C10H22	001072-16-8	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110921\
Data File : VX025116.D
Acq On : 09 Nov 2021 13:00
Operator : JC/MD
Sample : M4464-12ME 10X
Misc : 7.38g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GB7LOME

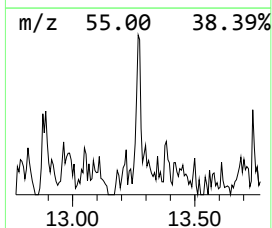
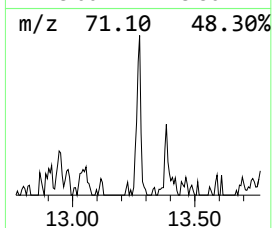
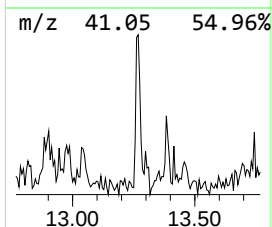
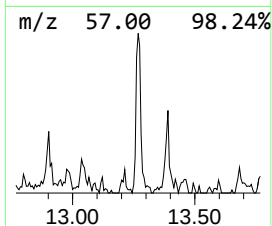
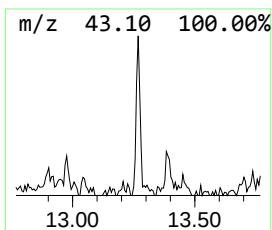
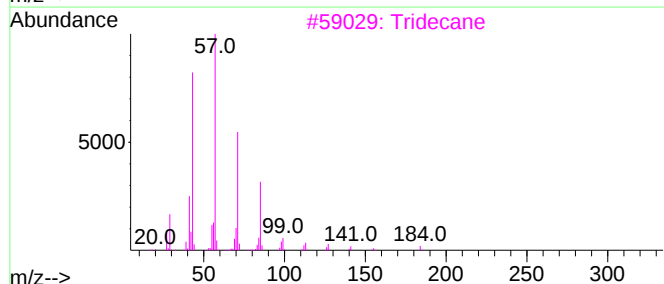
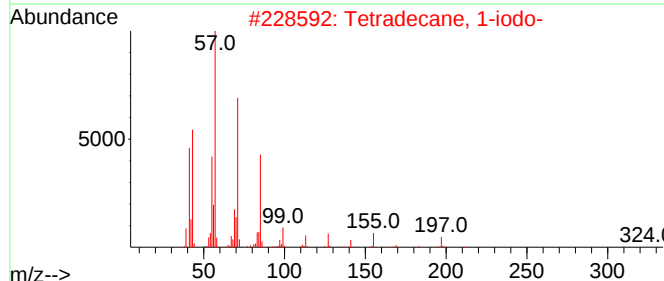
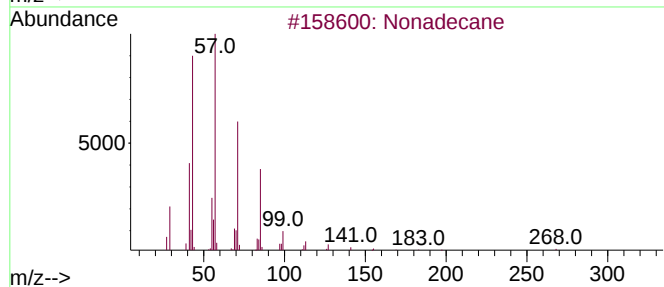
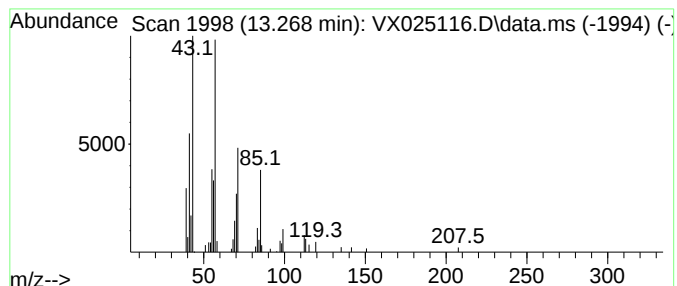
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Quant Title : VOC Analysis

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.268	3.75 ug/L	31466	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	72
2			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	72
3			Tridecane	184	C13H28	000629-50-5	64
4			Tetradecane	198	C14H30	000629-59-4	64
5			Tridecane	184	C13H28	000629-50-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110921\
Data File : VX025116.D
Acq On : 09 Nov 2021 13:00
Operator : JC/MD
Sample : M4464-12ME 10X
Misc : 7.38g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GB7LOME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML110821WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Ethyl-oxetane	3.447	3.1	ug/L	24228	1	6.769	386267	50.0
(DEL) Alkane: S...	10.360	3.4	ug/L	31412	2	10.055	460319	50.0
unknown-01	10.787	3.2	ug/L	29628	2	10.055	460319	50.0
(DEL) Alkane: S...	11.482	13.5	ug/L	113429	3	12.024	419954	50.0
(DEL) Alkane: S...	12.427	8.2	ug/L	68411	3	12.024	419954	50.0
(DEL) Alkane: S...	13.268	3.8	ug/L	31466	3	12.024	419954	50.0