

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
 Data File : VX025616.D
 Acq On : 08 Dec 2021 13:16
 Operator : JC/MD
 Sample : M4884-06ME
 Misc : 3.48g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EW9J2ME

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\SFAMXML112221WMA.M
 Title : VOC Analysis

Signal : TIC: VX025616.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	32	rBV2	4060	8417	2.10%	0.257%
2	1.368	43	46	55	rVB	46512	54311	13.56%	1.658%
3	1.563	70	78	79	rBV2	3908	8007	2.00%	0.244%
4	1.648	88	92	99	rBV	28797	34300	8.56%	1.047%
5	2.203	181	183	190	rVB3	902	1368	0.34%	0.042%
6	2.282	190	196	206	rBV	80014	132662	33.12%	4.049%
7	2.367	207	210	215	rVB2	919	1638	0.41%	0.050%
8	2.477	226	228	237	rVB2	276	565	0.14%	0.017%
9	2.569	242	243	246	rBV	101	124	0.03%	0.004%
10	2.648	251	256	257	rVV2	111	182	0.05%	0.006%
11	2.691	260	263	265	rVV2	356	463	0.12%	0.014%
12	2.733	268	270	273	rVV2	208	280	0.07%	0.009%
13	2.788	273	279	285	rVV6	1317	2874	0.72%	0.088%
14	2.837	285	287	291	rVB2	130	138	0.03%	0.004%
15	2.953	298	306	319	rBV	8132	23563	5.88%	0.719%
16	3.075	322	326	331	rVV5	772	1688	0.42%	0.052%
17	3.117	331	333	338	rVB2	353	404	0.10%	0.012%
18	3.404	377	380	383	rBV	114	155	0.04%	0.005%
19	3.757	434	438	443	rVB2	141	259	0.06%	0.008%
20	3.806	443	446	449	rVB2	143	141	0.04%	0.004%
21	3.831	449	450	452	rBV	173	131	0.03%	0.004%
22	4.105	492	495	498	rBV	138	168	0.04%	0.005%
23	4.288	517	525	526	rBV2	937	1368	0.34%	0.042%
24	4.495	546	559	583	rBV2	17702	85828	21.43%	2.620%
25	5.068	639	653	671	rBV3	46054	160489	40.06%	4.898%
26	5.446	712	715	716	rBV	523	518	0.13%	0.016%
27	5.544	729	731	732	rBV	315	260	0.06%	0.008%
28	5.836	778	779	781	rBV	387	194	0.05%	0.006%
29	5.970	790	801	818	rBV2	138085	400596	100.00%	12.227%
30	6.105	822	823	825	rBV	296	155	0.04%	0.005%
31	6.367	858	866	867	rBV4	2177	4498	1.12%	0.137%
32	6.763	922	931	947	rVB	89451	229136	57.20%	6.994%
33	7.104	983	987	990	rBV3	1180	2160	0.54%	0.066%
34	7.220	1002	1006	1008	rBV2	801	1093	0.27%	0.033%
35	7.312	1013	1021	1038	rVB	76757	187242	46.74%	5.715%
36	8.330	1182	1188	1198	rBV	42166	77388	19.32%	2.362%

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Integrator: RTE

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37	8.653	1234	1241	1248	rBV	189925	316288	78.95%	9.654%
38	8.720	1248	1252	1260	rVB	4121	6485	1.62%	0.198%
39	8.958	1285	1291	1304	rBV	28536	50342	12.57%	1.537%
40	9.397	1357	1363	1376	rBV	107544	186113	46.46%	5.680%
41	9.561	1388	1390	1395	rVB2	1035	1054	0.26%	0.032%
42	9.714	1412	1415	1419	rVB3	1406	1953	0.49%	0.060%
43	10.061	1466	1472	1486	rBV	179000	267478	66.77%	8.164%
44	10.201	1491	1495	1500	rVB2	811	1082	0.27%	0.033%
45	10.305	1508	1512	1518	rVB2	3553	4983	1.24%	0.152%
46	10.354	1518	1520	1524	rBV3	682	803	0.20%	0.025%
47	10.646	1564	1568	1574	rVB	3671	5279	1.32%	0.161%
48	10.963	1618	1620	1624	rVB2	1213	1197	0.30%	0.037%
49	11.122	1642	1646	1650	rVB	1966	2677	0.67%	0.082%
50	11.201	1653	1659	1665	rBV	142735	192359	48.02%	5.871%
51	11.311	1674	1677	1684	rVB4	1899	2956	0.74%	0.090%
52	11.384	1686	1689	1694	rVB2	1239	1720	0.43%	0.052%
53	11.476	1702	1704	1708	rVB2	1630	1846	0.46%	0.056%
54	11.616	1724	1727	1734	rVB3	881	1348	0.34%	0.041%
55	11.719	1741	1744	1746	rBV2	776	915	0.23%	0.028%
56	11.750	1746	1749	1755	rVB3	4495	6404	1.60%	0.195%
57	11.841	1762	1764	1766	rVB2	486	327	0.08%	0.010%
58	11.939	1776	1780	1783	rVB4	1170	1671	0.42%	0.051%
59	11.976	1784	1786	1789	rBV	443	305	0.08%	0.009%
60	12.024	1789	1794	1800	rBV	214491	263527	65.78%	8.043%
61	12.128	1809	1811	1812	rBV	804	525	0.13%	0.016%
62	12.152	1812	1815	1822	rVB3	1681	2462	0.61%	0.075%
63	12.225	1825	1827	1829	rVB2	638	490	0.12%	0.015%
64	12.323	1838	1843	1851	rVB	231573	289836	72.35%	8.846%
65	12.427	1856	1860	1864	rVB2	5237	6048	1.51%	0.185%
66	12.469	1864	1867	1872	rVB5	1025	1631	0.41%	0.050%
67	12.555	1879	1881	1882	rBV2	339	249	0.06%	0.008%
68	12.616	1889	1891	1896	rVV3	405	489	0.12%	0.015%
69	12.658	1896	1898	1900	rVV	494	576	0.14%	0.018%
70	12.683	1900	1902	1905	rVB	974	1051	0.26%	0.032%
71	12.725	1905	1909	1913	rBV3	507	948	0.24%	0.029%
72	12.768	1913	1916	1919	rVB2	773	965	0.24%	0.029%
73	12.847	1927	1929	1931	rBV	481	518	0.13%	0.016%
74	12.981	1947	1951	1954	rVB2	1445	2013	0.50%	0.061%
75	13.042	1958	1961	1967	rVB5	887	1606	0.40%	0.049%
76	13.085	1967	1968	1972	rBV3	391	467	0.12%	0.014%

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Instrument :
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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Stop Thrs : 0

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Peak separation: 5

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 Title : VOC Analysis

77	13.213	1985	1989	1993	rBV3	883	1304	0.33%	0.040%
78	13.268	1994	1998	2008	rVV2	10953	14921	3.72%	0.455%
79	13.384	2014	2017	2021	rBV	4584	5581	1.39%	0.170%
80	13.591	2047	2051	2052	rBV2	694	1072	0.27%	0.033%
81	13.683	2064	2066	2067	rBV	863	562	0.14%	0.017%
82	13.701	2067	2069	2071	rVV3	1775	1711	0.43%	0.052%
83	13.737	2073	2075	2078	rVB2	2244	2100	0.52%	0.064%
84	13.774	2078	2081	2088	rVB2	5100	8088	2.02%	0.247%
85	13.841	2088	2092	2099	rBV	9945	13016	3.25%	0.397%
86	13.902	2099	2102	2103	rBV3	1156	1350	0.34%	0.041%
87	13.993	2114	2117	2119	rBV3	1344	1704	0.43%	0.052%
88	14.042	2121	2125	2128	rVV	23704	27432	6.85%	0.837%
89	14.134	2137	2140	2144	rVB3	4053	4686	1.17%	0.143%
90	14.189	2147	2149	2153	rVB3	2925	3025	0.76%	0.092%
91	14.414	2183	2186	2192	rBV6	2287	4873	1.22%	0.149%
92	14.469	2193	2195	2198	rBV3	1868	1781	0.44%	0.054%
93	14.506	2198	2201	2207	rVB4	5081	8234	2.06%	0.251%
94	14.567	2208	2211	2215	rVB3	3231	4398	1.10%	0.134%
95	14.615	2215	2219	2222	rBV	14830	18465	4.61%	0.564%
96	14.755	2238	2242	2245	rBV	30197	34448	8.60%	1.051%
97	15.213	2314	2317	2324	rVB	16172	21060	5.26%	0.643%
98	15.274	2325	2327	2332	rVB4	3380	4435	1.11%	0.135%
99	15.493	2359	2363	2368	rVB2	15502	20521	5.12%	0.626%
100	16.383	2503	2509	2514	rBV2	11287	19857	4.96%	0.606%

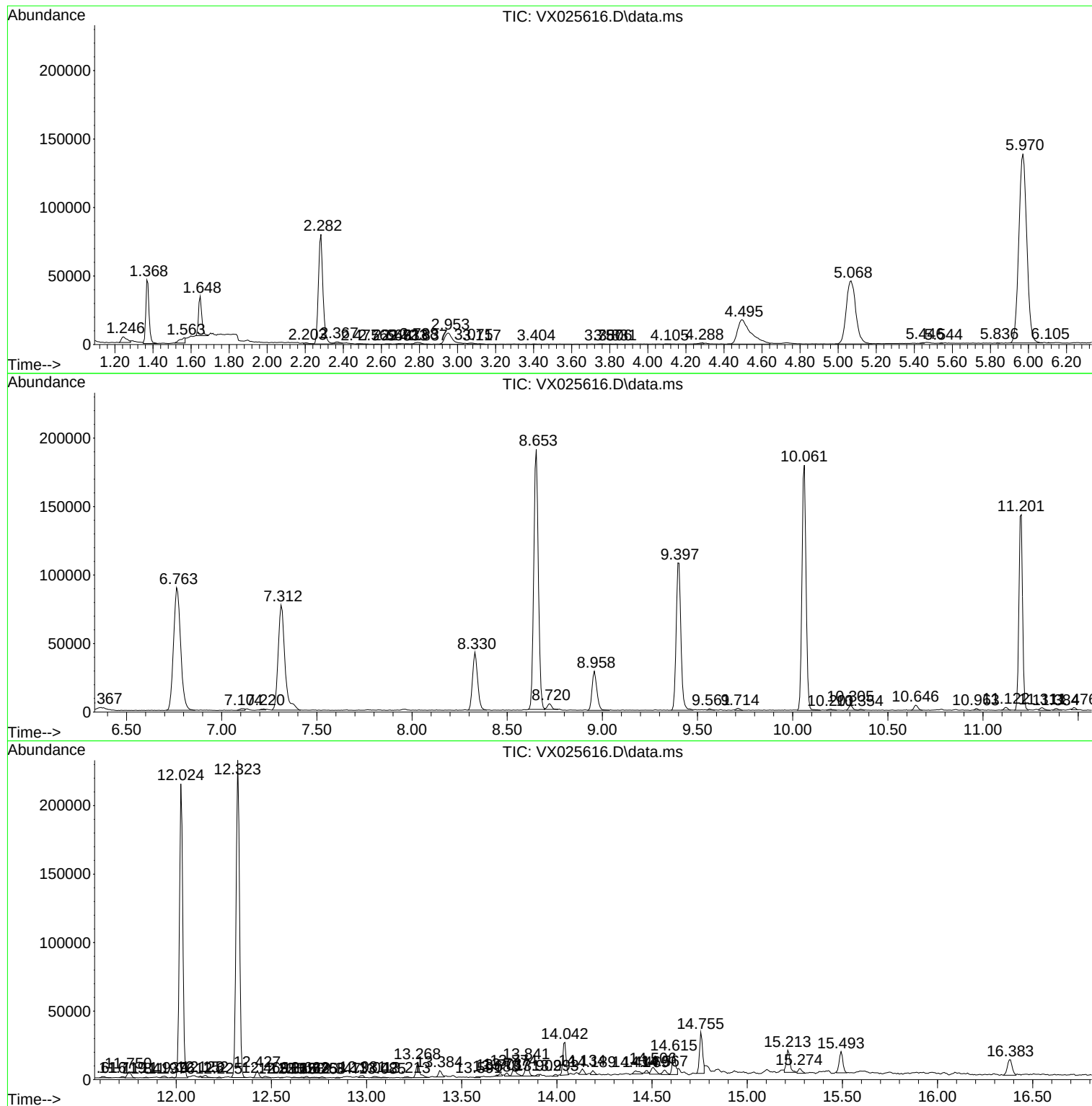
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Instrument :
MSVOA_X
ClientSampleId :
EW9J2ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML112221WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_X
ClientSampleId :
EW9J2ME

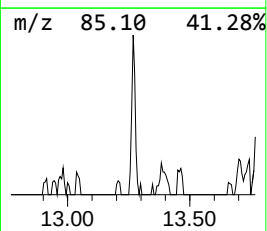
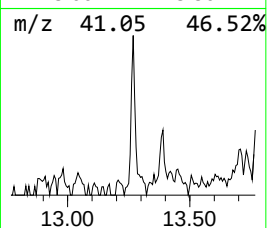
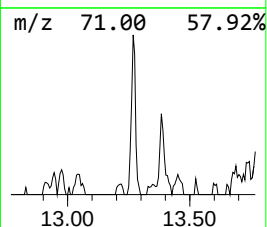
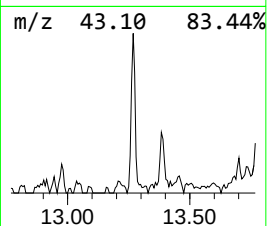
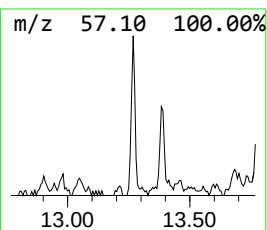
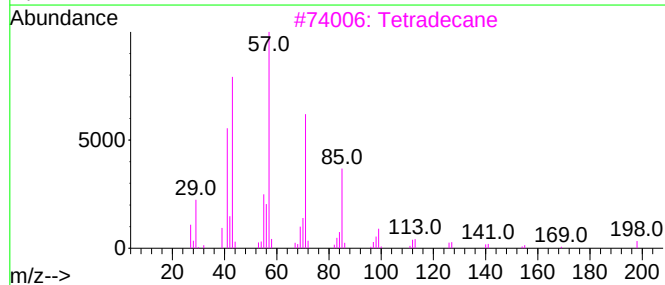
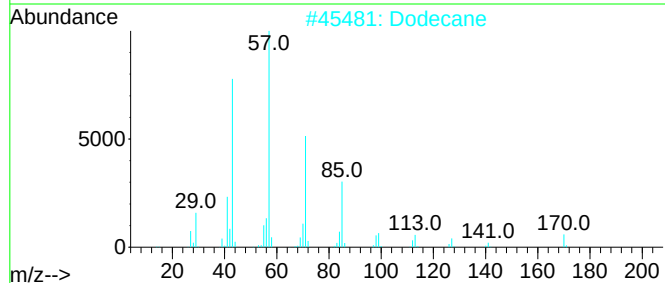
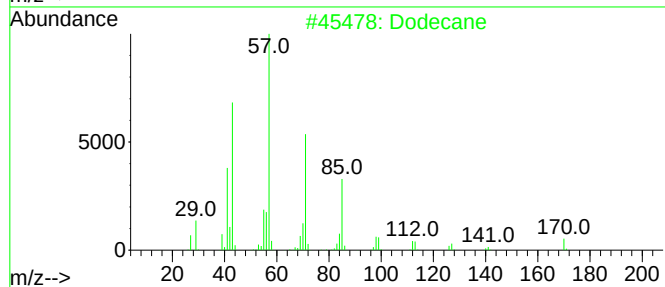
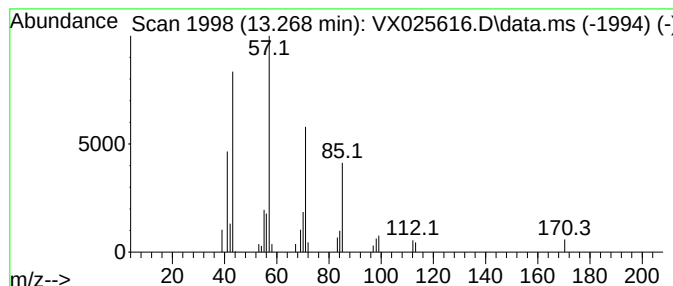
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.268	2.83 ug/L	14921	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	90
3			Tetradecane	198	C14H30	000629-59-4	90
4			Hexadecane	226	C16H34	000544-76-3	90
5			Heptadecane	240	C17H36	000629-78-7	86



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ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9J2ME

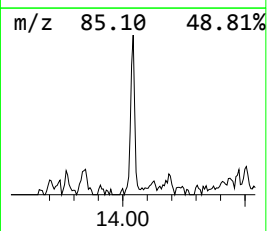
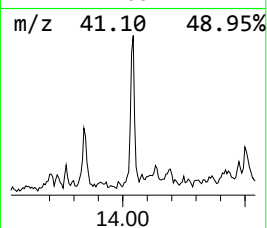
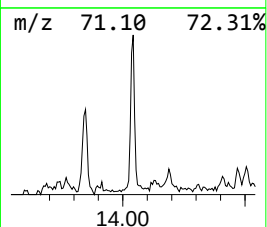
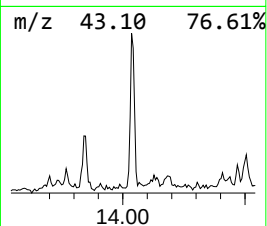
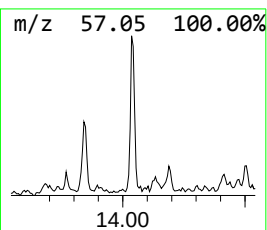
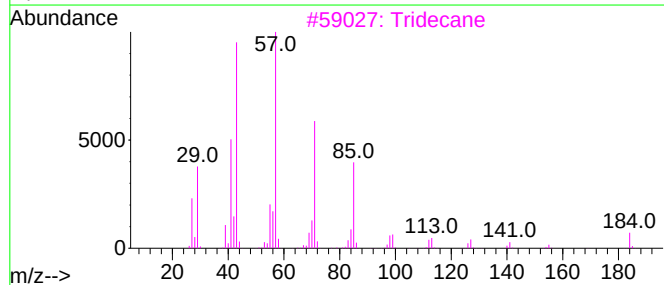
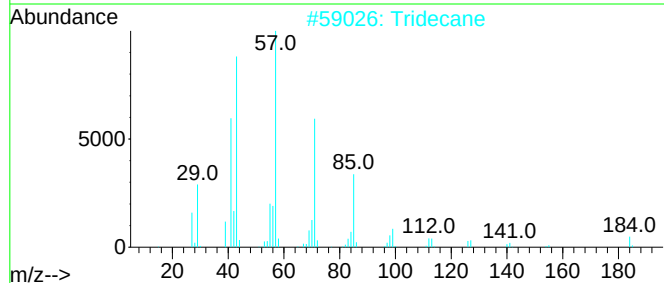
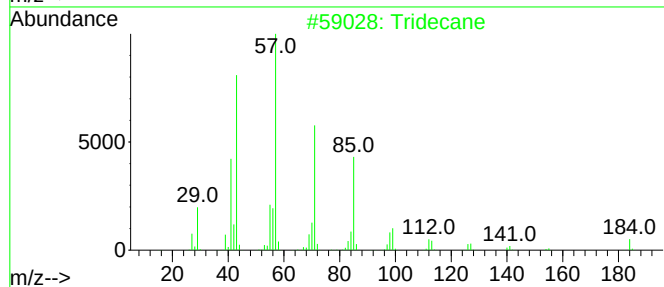
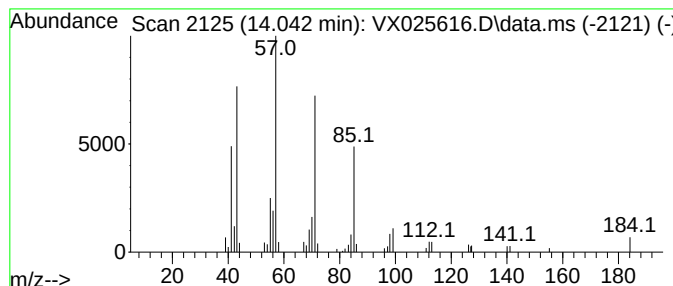
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.042	5.20 ug/L	27432	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	97
2			Tridecane	184	C13H28	000629-50-5	95
3			Tridecane	184	C13H28	000629-50-5	94
4			Pentadecane	212	C15H32	000629-62-9	90
5			Dodecane	170	C12H26	000112-40-3	90



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ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9J2ME

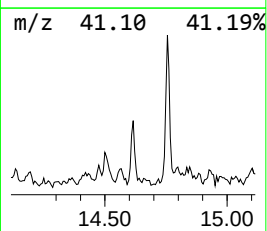
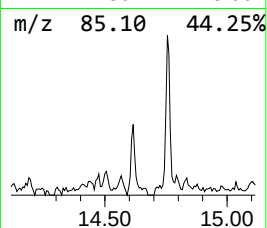
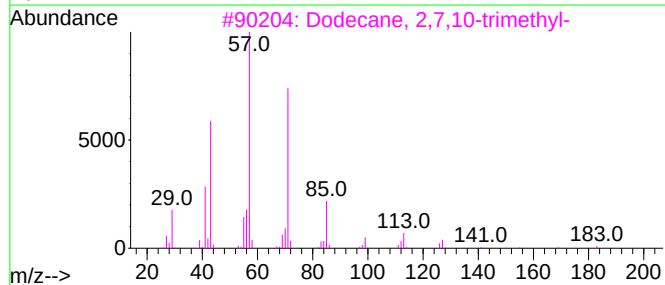
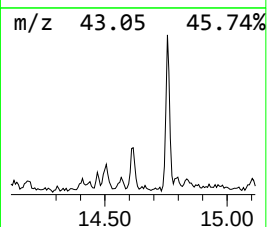
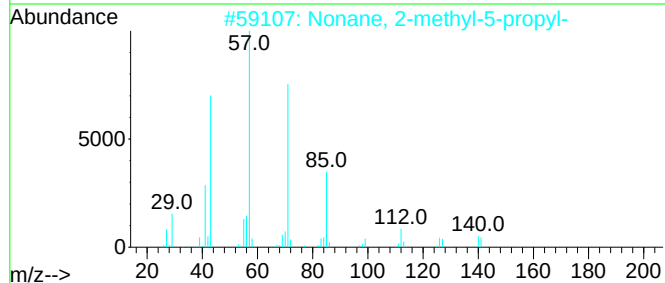
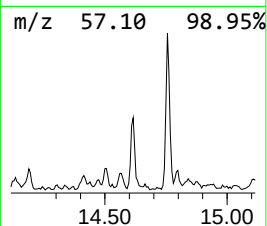
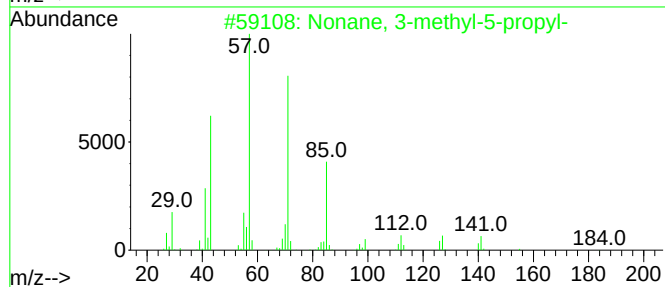
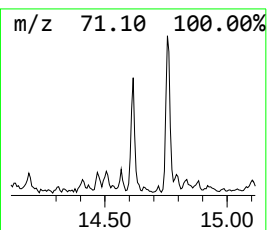
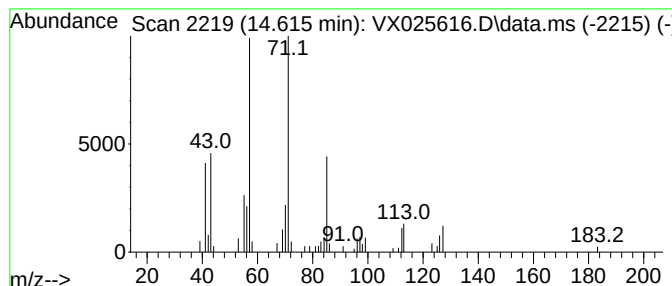
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.615	3.50 ug/L	18465	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	72
2		Nonane, 2-methyl-5-propyl-	184	C13H28	031081-17-1	64
3		Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	59
4		Decane, 5-propyl-	184	C13H28	017312-62-8	59
5		Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
Data File : VX025616.D
Acq On : 08 Dec 2021 13:16
Operator : JC/MD
Sample : M4884-06ME
Misc : 3.48g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9J2ME

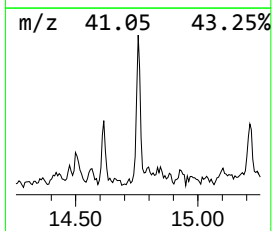
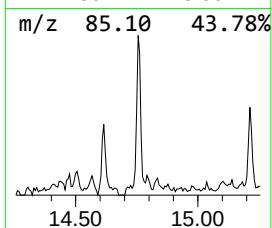
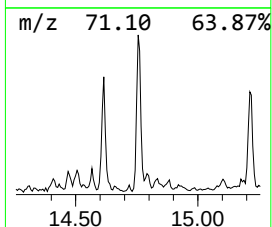
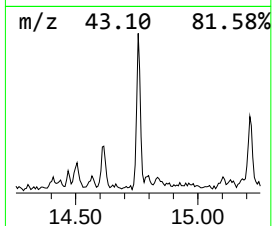
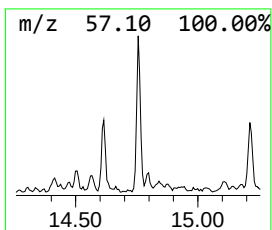
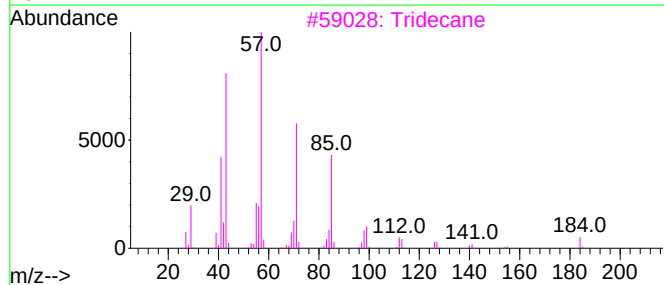
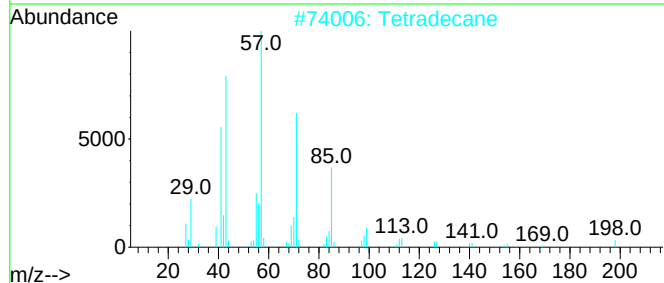
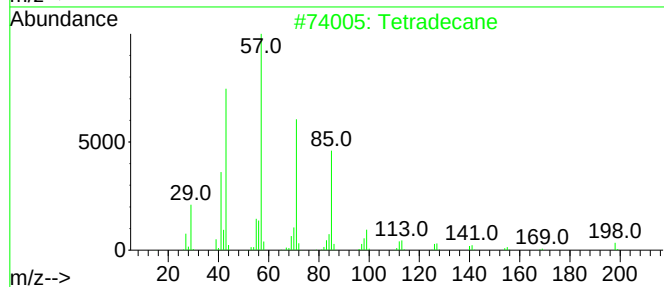
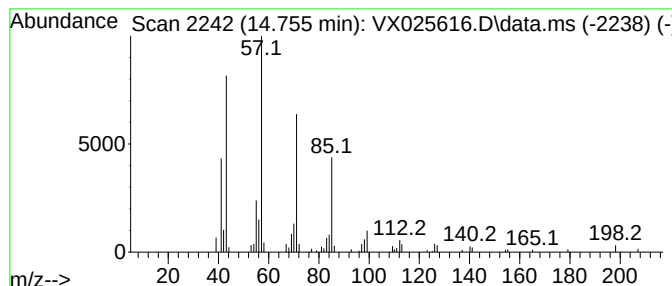
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Quant Title : VOC Analysis

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.756	6.54 ug/L	34448	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	97
2			Tetradecane	198	C14H30	000629-59-4	96
3			Tridecane	184	C13H28	000629-50-5	90
4			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	86
5			Pentadecane	212	C15H32	000629-62-9	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
Data File : VX025616.D
Acq On : 08 Dec 2021 13:16
Operator : JC/MD
Sample : M4884-06ME
Misc : 3.48g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9J2ME

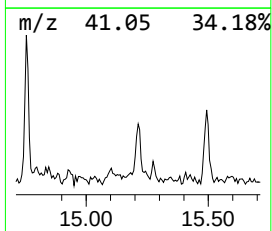
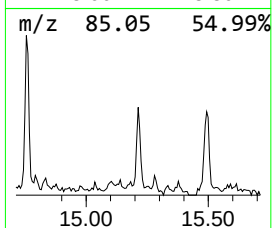
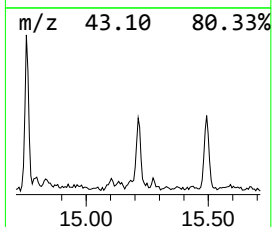
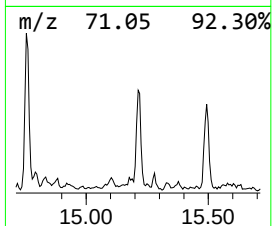
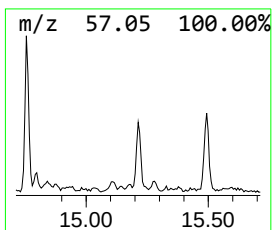
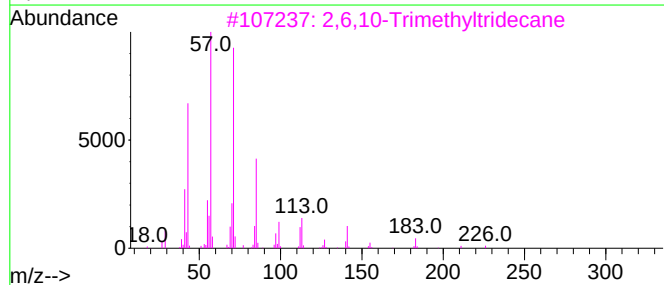
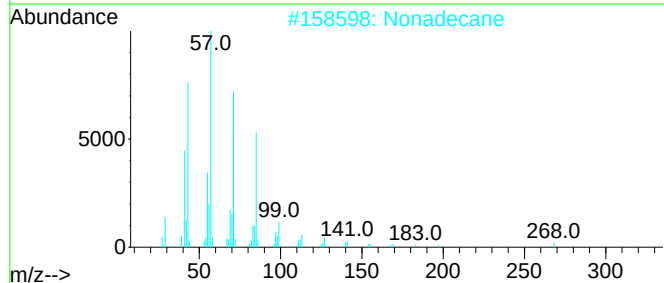
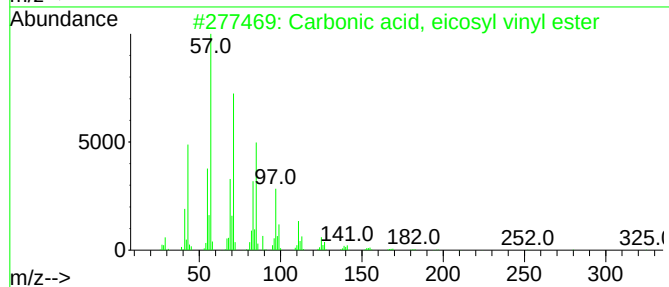
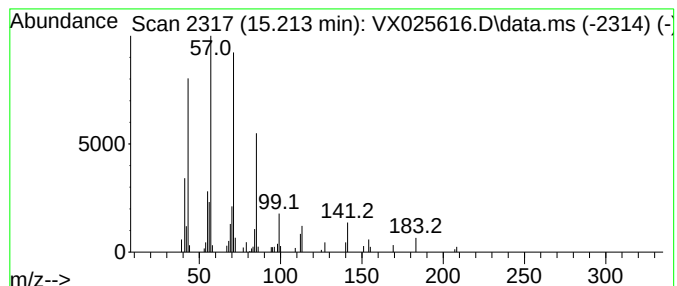
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Quant Title : VOC Analysis

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

Peak Number 7 Carbonic acid, eicosyl vinyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.213	4.00 ug/L	21060	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	90
2			Nonadecane	268	C19H40	000629-92-5	83
3			2,6,10-Trimethyltridecane	226	C16H34	003891-99-4	80
4			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	72
5			3-Ethyl-2,6,10-trimethylundecane	226	C16H34	1000432-25-9	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
Data File : VX025616.D
Acq On : 08 Dec 2021 13:16
Operator : JC/MD
Sample : M4884-06ME
Misc : 3.48g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9J2ME

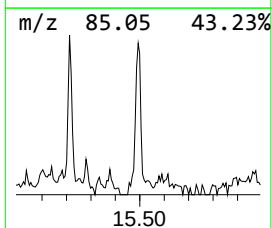
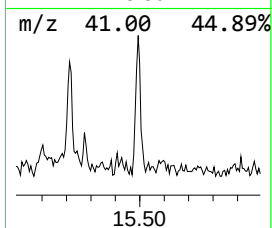
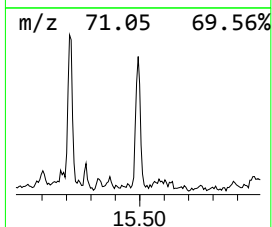
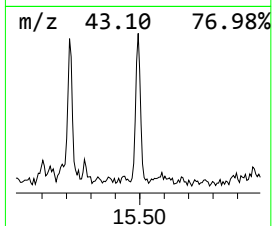
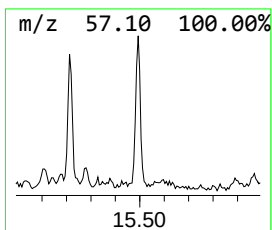
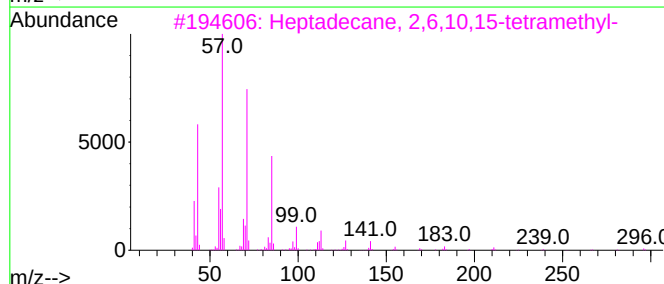
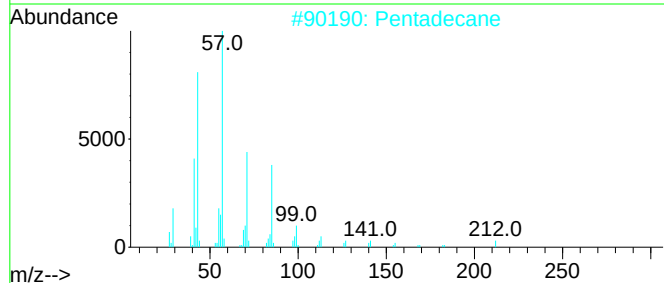
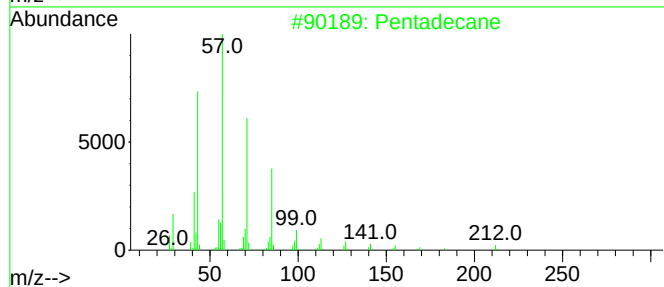
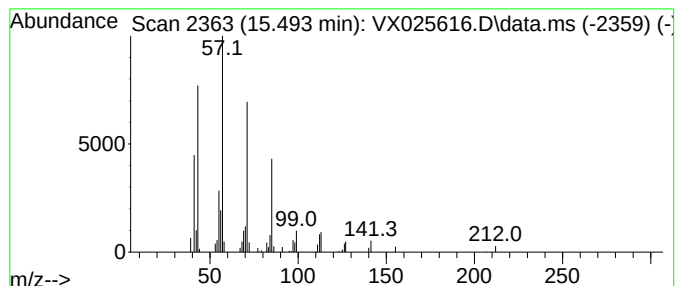
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Quant Title : VOC Analysis

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.493	3.89 ug/L	20521	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane	212	C15H32	000629-62-9	96
2			Pentadecane	212	C15H32	000629-62-9	95
3			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
4			Pentadecane	212	C15H32	000629-62-9	90
5			Tetradecane	198	C14H30	000629-59-4	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
Data File : VX025616.D
Acq On : 08 Dec 2021 13:16
Operator : JC/MD
Sample : M4884-06ME
Misc : 3.48g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9J2ME

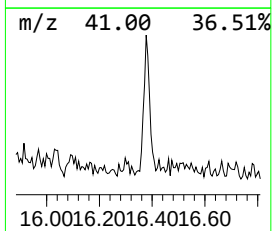
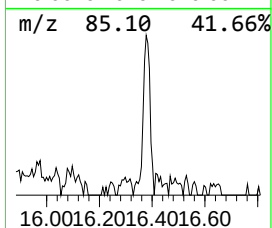
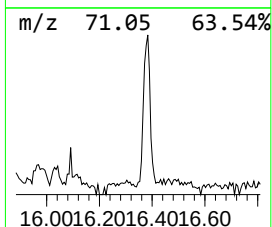
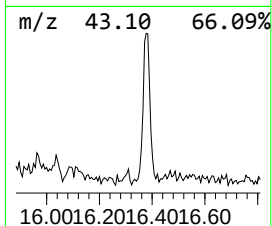
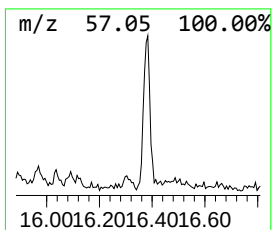
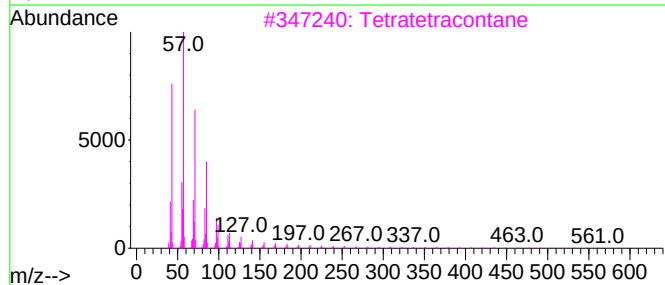
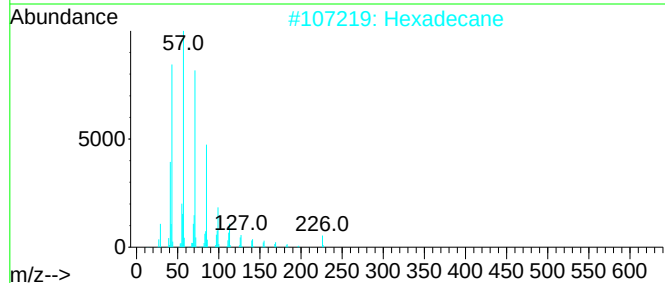
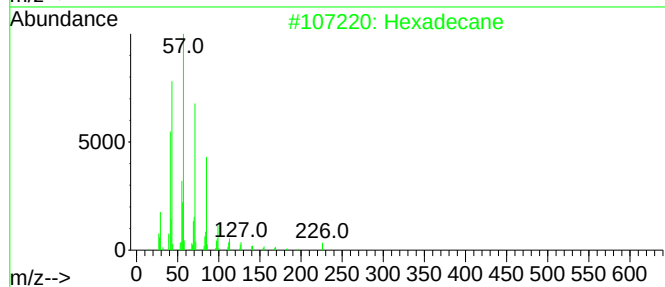
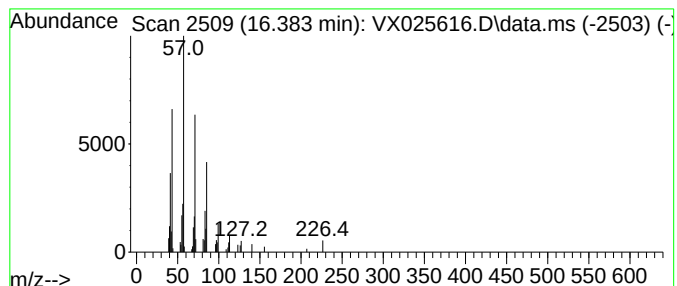
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Quant Title : VOC Analysis

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

Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.383	3.77 ug/L	19857	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	96
2			Hexadecane	226	C16H34	000544-76-3	92
3			Tetratetracontane	619	C44H90	007098-22-8	90
4			Hexadecane	226	C16H34	000544-76-3	81
5			Heptadecane	240	C17H36	000629-78-7	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
Data File : VX025616.D
Acq On : 08 Dec 2021 13:16
Operator : JC/MD
Sample : M4884-06ME
Misc : 3.48g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9J2ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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

						--Internal Standard--			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc	
(DEL) Alkane: S...	13.268	2.8	ug/L	14921	3	12.024	263527	50.0	
(DEL) Alkane: S...	14.042	5.2	ug/L	27432	3	12.024	263527	50.0	
(DEL) Alkane: S...	14.615	3.5	ug/L	18465	3	12.024	263527	50.0	
(DEL) Alkane: S...	14.756	6.5	ug/L	34448	3	12.024	263527	50.0	
Carbonic acid, ...	15.213	4.0	ug/L	21060	3	12.024	263527	50.0	
(DEL) Alkane: S...	15.493	3.9	ug/L	20521	3	12.024	263527	50.0	
(DEL) Alkane: S...	16.383	3.8	ug/L	19857	3	12.024	263527	50.0	