

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051022\
 Data File : VU048482.D
 Acq On : 10 May 2022 11:44
 Operator : SY/MD
 Sample : N2708-07ME
 Misc : 4.78g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXL33ME

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_U\Method\SFAMULM050622WMA.M
 Title : VOC Analysis

Signal : TIC: VU048482.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.478	36	43	66	rVB	263277	342993	28.75%	2.715%
2	1.597	73	80	104	rVB	91891	163431	13.70%	1.293%
3	2.237	275	279	282	rBV4	1381	1266	0.11%	0.010%
4	2.536	361	372	384	rBV	282815	454330	38.08%	3.596%
5	2.636	394	403	428	rVB2	75278	148067	12.41%	1.172%
6	2.954	491	502	513	rBV	22790	45854	3.84%	0.363%
7	3.176	556	571	590	rBV	39059	94329	7.91%	0.747%
8	3.327	615	618	619	rBV2	1186	715	0.06%	0.006%
9	3.571	685	694	707	rVB8	3054	7128	0.60%	0.056%
10	4.076	839	851	856	rVB4	1207	2561	0.21%	0.020%
11	4.507	977	985	988	rBV8	2406	3467	0.29%	0.027%
12	4.632	1010	1024	1037	rBV	111051	311212	26.09%	2.463%
13	4.710	1041	1048	1072	rVB	154614	413186	34.63%	3.270%
14	5.060	1140	1157	1185	rBV2	254346	600756	50.36%	4.755%
15	5.195	1188	1199	1221	rVV	51726	116796	9.79%	0.924%
16	5.443	1272	1276	1289	rVB5	1791	2833	0.24%	0.022%
17	5.575	1313	1317	1329	rVB6	1273	1845	0.15%	0.015%
18	5.719	1340	1362	1387	rBV3	457569	1192974	100.00%	9.442%
19	5.912	1413	1422	1429	rVV5	1039	1619	0.14%	0.013%
20	5.976	1429	1442	1469	rVV4	14798	37912	3.18%	0.300%
21	6.163	1481	1500	1512	rVV2	18920	54845	4.60%	0.434%
22	6.247	1513	1526	1553	rVB	445200	911746	76.43%	7.216%
23	6.398	1559	1573	1593	rBV2	44329	97714	8.19%	0.773%
24	6.526	1605	1613	1624	rVB9	3799	6837	0.57%	0.054%
25	6.600	1624	1636	1648	rBV4	8015	18995	1.59%	0.150%
26	6.687	1650	1663	1678	rVV	251783	506314	42.44%	4.007%
27	6.774	1680	1690	1720	rVB4	35872	128170	10.74%	1.014%
28	6.928	1726	1738	1767	rBV	29897	92511	7.75%	0.732%
29	7.063	1776	1780	1783	rBV5	783	727	0.06%	0.006%
30	7.185	1806	1818	1850	rBV4	84981	208882	17.51%	1.653%
31	7.378	1868	1878	1893	rVB6	4097	8274	0.69%	0.065%
32	7.494	1909	1914	1923	rVB8	1947	2727	0.23%	0.022%
33	7.568	1923	1937	1958	rBV	138323	271929	22.79%	2.152%
34	7.693	1970	1976	1985	rVB5	1522	2204	0.18%	0.017%
35	7.787	1999	2005	2007	rBV3	1695	1770	0.15%	0.014%
36	7.896	2027	2039	2054	rBV	450701	803629	67.36%	6.360%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
 Title : VOC Analysis

37	7.967	2056	2061	2078	rVB2	16839	30392	2.55%	0.241%
38	8.037	2080	2083	2089	rVB5	2957	2722	0.23%	0.022%
39	8.182	2117	2128	2156	rVB3	112614	244135	20.46%	1.932%
40	8.472	2215	2218	2228	rVB4	1254	1822	0.15%	0.014%
41	8.552	2233	2243	2256	rVB3	15262	25690	2.15%	0.203%
42	8.655	2258	2275	2301	rBV	276217	654158	54.83%	5.177%
43	8.803	2310	2321	2330	rVB7	3367	6909	0.58%	0.055%
44	8.864	2333	2340	2350	rVB8	1752	2747	0.23%	0.022%
45	8.925	2350	2359	2369	rBV5	5360	8895	0.75%	0.070%
46	9.118	2413	2419	2423	rBV3	1815	1901	0.16%	0.015%
47	9.214	2445	2449	2456	rVB6	677	883	0.07%	0.007%
48	9.420	2499	2513	2532	rBV	533432	999078	83.75%	7.907%
49	9.574	2549	2561	2576	rVB4	4169	7930	0.66%	0.063%
50	9.693	2587	2598	2608	rVV2	12211	21575	1.81%	0.171%
51	9.745	2609	2614	2624	rVV4	4227	5132	0.43%	0.041%
52	10.105	2716	2726	2741	rBV4	9573	17657	1.48%	0.140%
53	10.246	2758	2770	2772	rBV5	1953	2482	0.21%	0.020%
54	10.391	2809	2815	2826	rVB4	1921	3035	0.25%	0.024%
55	10.481	2833	2843	2853	rVB7	2858	5268	0.44%	0.042%
56	10.558	2859	2867	2873	rBV5	943	1268	0.11%	0.010%
57	10.661	2891	2899	2904	rBV8	2152	3544	0.30%	0.028%
58	10.764	2917	2931	2947	rBV	364601	600209	50.31%	4.750%
59	10.828	2947	2951	2959	rVB4	1316	1257	0.11%	0.010%
60	10.896	2960	2972	2988	rBV	34683	57559	4.82%	0.456%
61	10.999	2998	3004	3006	rBV3	1398	1180	0.10%	0.009%
62	11.012	3006	3008	3012	rVV	1380	950	0.08%	0.008%
63	11.057	3015	3022	3029	rVV3	21890	31792	2.66%	0.252%
64	11.115	3029	3040	3054	rVB	296519	422372	35.40%	3.343%
65	11.208	3066	3069	3072	rVB3	923	632	0.05%	0.005%
66	11.301	3088	3098	3101	rBV6	3122	4558	0.38%	0.036%
67	11.375	3115	3121	3127	rBV6	2634	3509	0.29%	0.028%
68	11.417	3127	3134	3141	rVV4	5451	8005	0.67%	0.063%
69	11.471	3141	3151	3167	rVB3	12427	24389	2.04%	0.193%
70	11.571	3175	3182	3190	rBV5	3277	5134	0.43%	0.041%
71	11.642	3196	3204	3209	rBV6	1938	2386	0.20%	0.019%
72	11.693	3213	3220	3228	rBV7	2011	3522	0.30%	0.028%
73	11.748	3230	3237	3243	rBV7	3423	4964	0.42%	0.039%
74	11.815	3246	3258	3271	rVV	741236	1162461	97.44%	9.200%
75	11.873	3272	3276	3281	rVV3	12947	17204	1.44%	0.136%
76	11.909	3283	3287	3296	rVB4	20885	27808	2.33%	0.220%

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 ClientSampleId :
 EXL33ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
 Title : VOC Analysis

77	12.002	3310	3316	3325	rVB2	16921	24257	2.03%	0.192%
78	12.195	3361	3376	3394	rBV	527658	855501	71.71%	6.771%
79	12.327	3407	3417	3427	rBV	64962	94060	7.88%	0.744%
80	12.465	3455	3460	3462	rBV4	1017	768	0.06%	0.006%
81	12.504	3467	3472	3476	rVB3	811	757	0.06%	0.006%
82	12.774	3546	3556	3565	rBV3	5894	8049	0.67%	0.064%
83	12.899	3586	3595	3601	rBV6	1881	3240	0.27%	0.026%
84	12.970	3612	3617	3618	rBV2	710	685	0.06%	0.005%
85	12.995	3623	3625	3627	rVV3	1308	766	0.06%	0.006%
86	13.041	3631	3639	3648	rVV6	2024	3545	0.30%	0.028%
87	13.137	3665	3669	3671	rBV4	807	644	0.05%	0.005%
88	13.221	3686	3695	3704	rBV8	4362	6705	0.56%	0.053%
89	13.391	3734	3748	3756	rBV3	34860	52694	4.42%	0.417%
90	13.430	3756	3760	3770	rVV3	8462	11121	0.93%	0.088%
91	13.584	3799	3808	3816	rBV4	2574	3806	0.32%	0.030%
92	13.848	3880	3890	3896	rBV6	4251	6688	0.56%	0.053%
93	14.092	3954	3966	3980	rBV	15822	26671	2.24%	0.211%
94	14.188	3988	3996	4004	rVB7	3251	5327	0.45%	0.042%
95	14.275	4020	4023	4026	rVB3	956	663	0.06%	0.005%
96	14.330	4034	4040	4052	rBV6	4099	6433	0.54%	0.051%
97	14.449	4069	4077	4087	rBB3	6145	8265	0.69%	0.065%
98	15.066	4264	4269	4274	rBV5	1327	1703	0.14%	0.013%
99	15.224	4308	4318	4330	rVB5	5153	11281	0.95%	0.089%
100	15.372	4356	4364	4370	rBV8	8987	13580	1.14%	0.107%

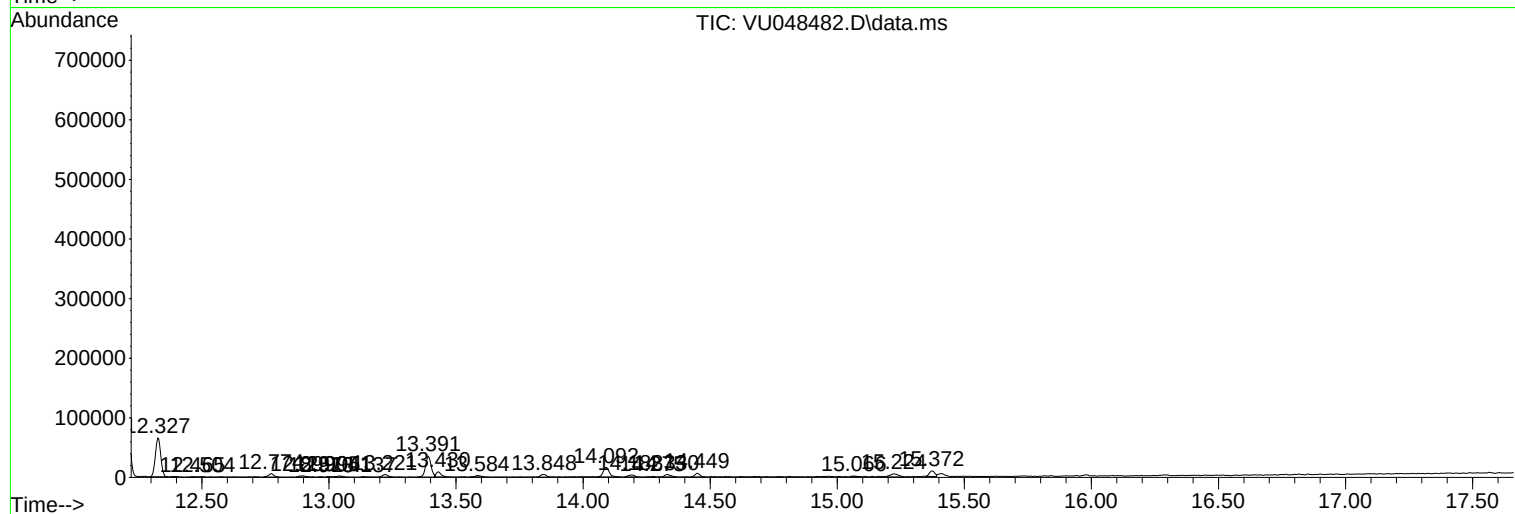
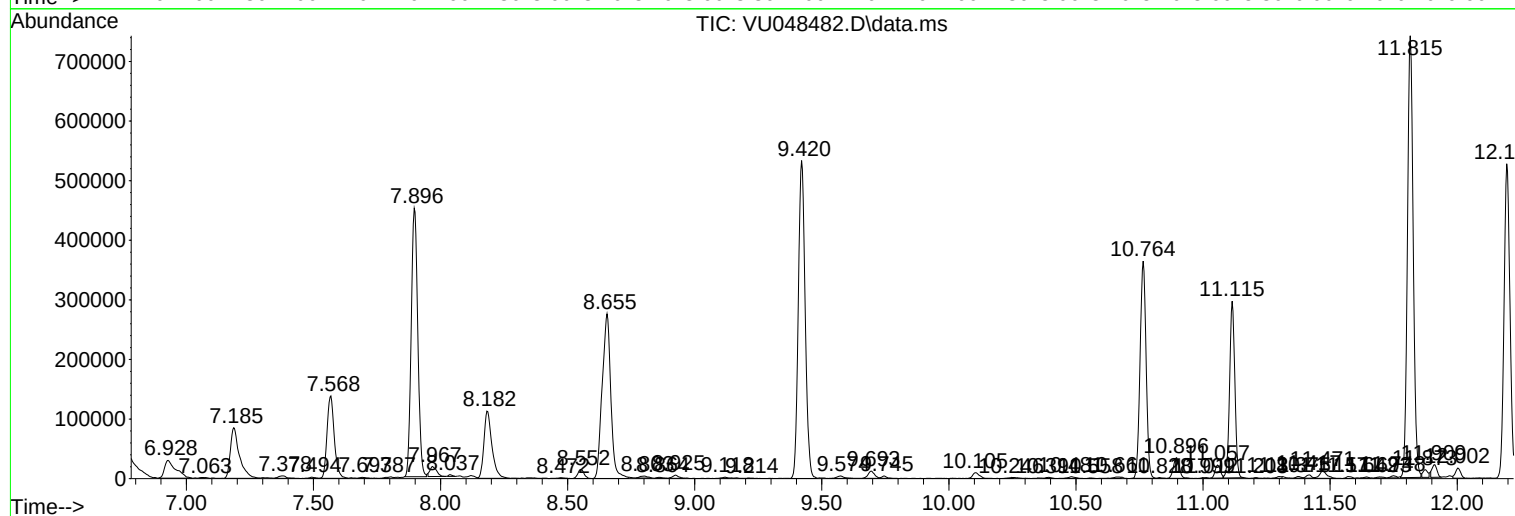
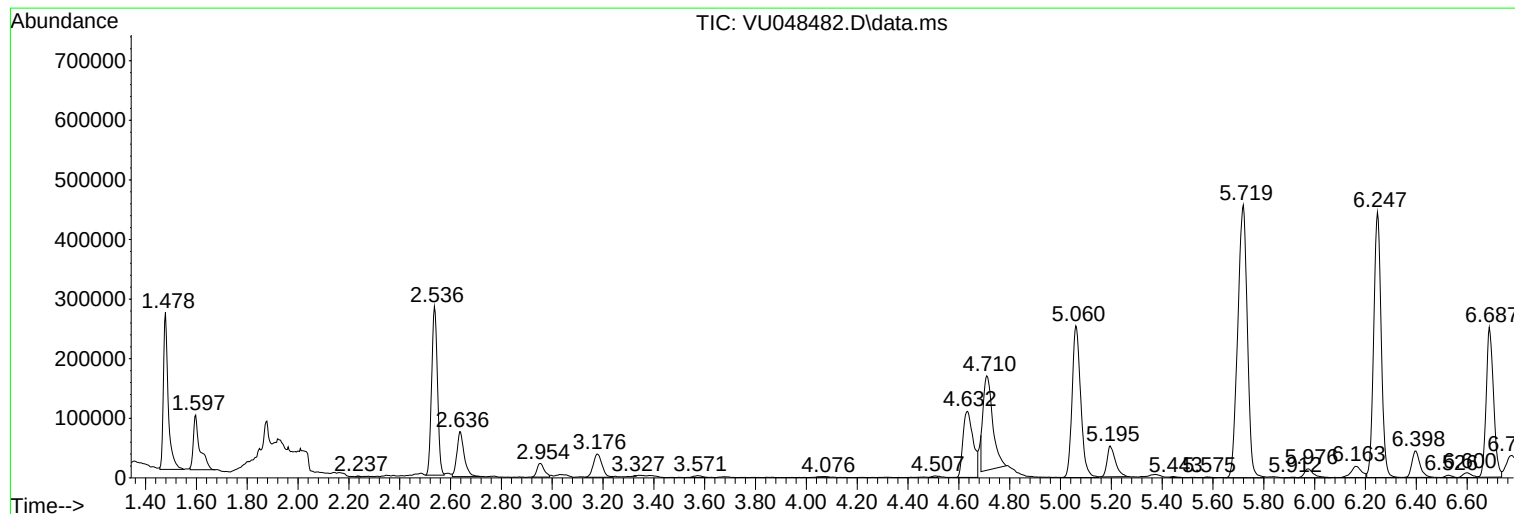
Sum of corrected areas: 12634871

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Instrument :
MSVOA_U
ClientSampleId :
EXL33ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_U
ClientSampleId :
EXL33ME

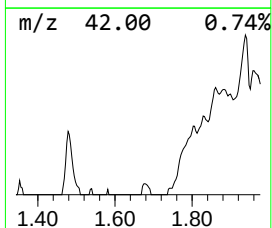
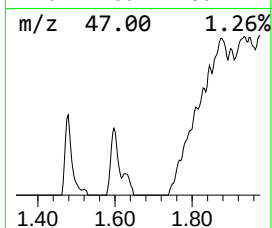
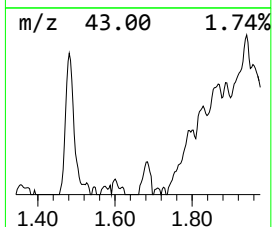
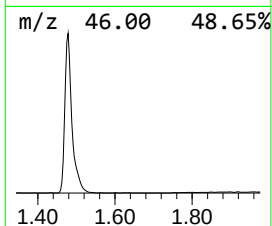
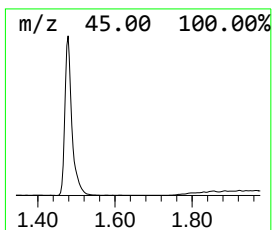
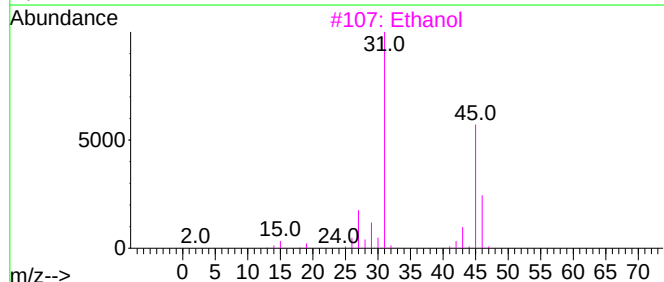
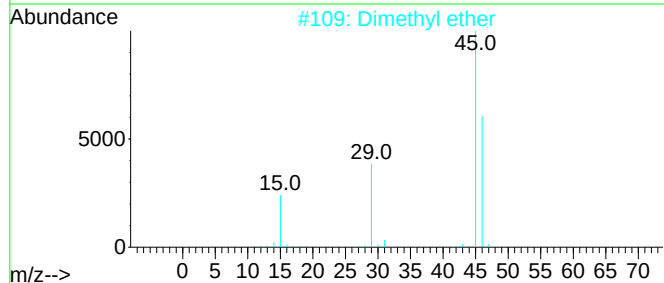
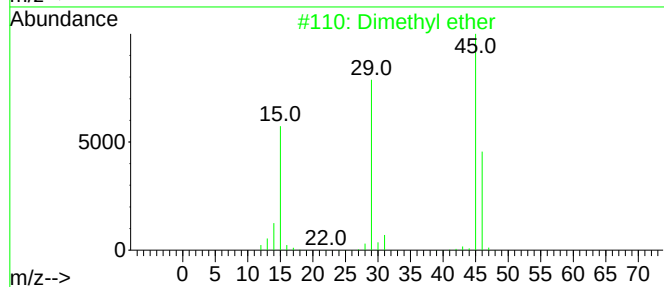
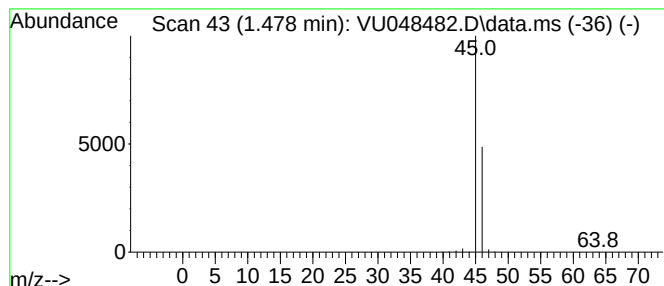
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Dimethyl ether Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.478	18.81 ug/L	342993	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl ether	46	C2H6O	000115-10-6	64
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Ethanol	46	C2H6O	000064-17-5	7
4			Ethanol	46	C2H6O	000064-17-5	7
5			Dimethyl ether	46	C2H6O	000115-10-6	5



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Instrument :
MSVOA_U
ClientSampleId :
EXL33ME

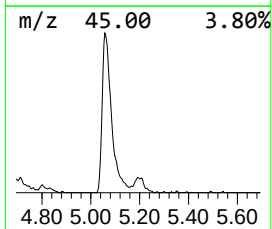
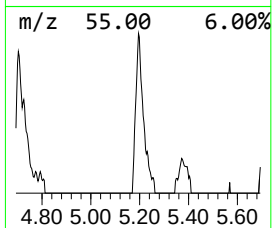
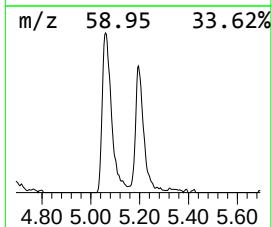
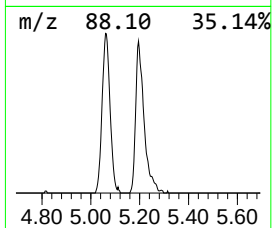
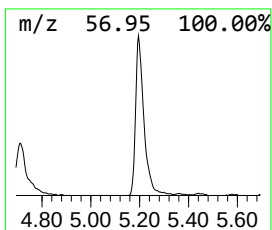
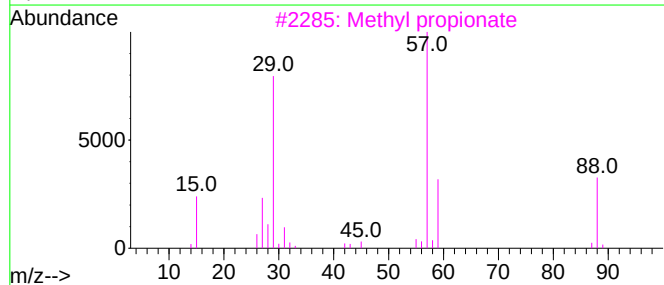
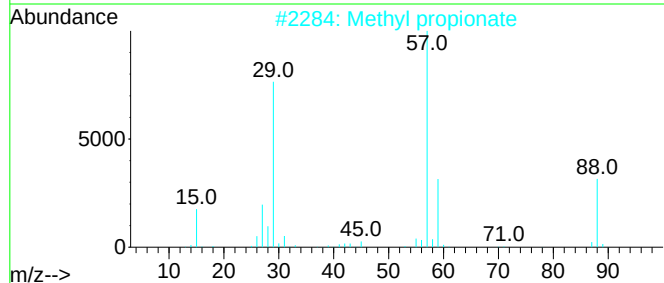
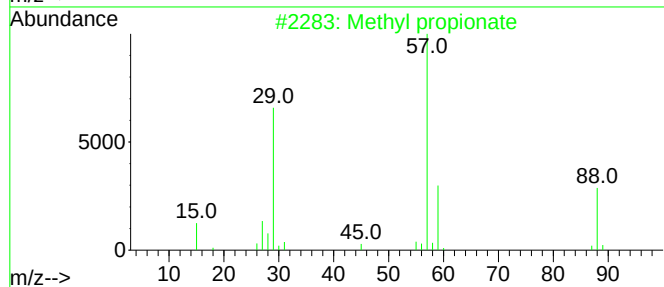
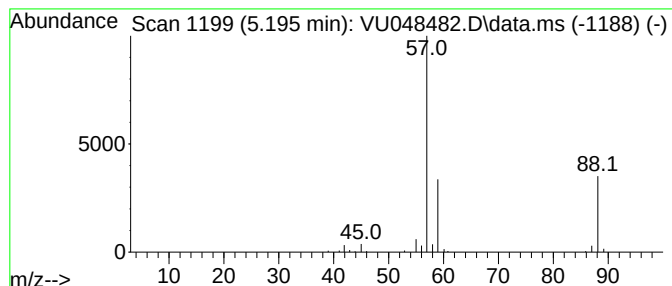
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Methyl propionate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.195	6.41 ug/L	116796	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl propionate			88	C4H8O2	000554-12-1	90
2	Methyl propionate			88	C4H8O2	000554-12-1	86
3	Methyl propionate			88	C4H8O2	000554-12-1	80
4	Methyl propionate			88	C4H8O2	000554-12-1	78
5	Methyl propionate			88	C4H8O2	000554-12-1	72



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ALS Vial : 6 Sample Multiplier: 1

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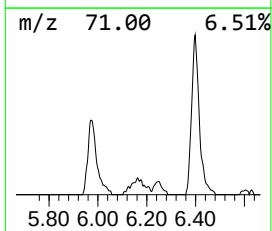
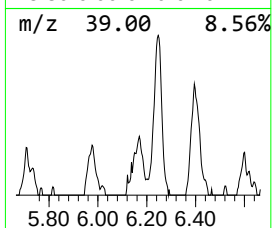
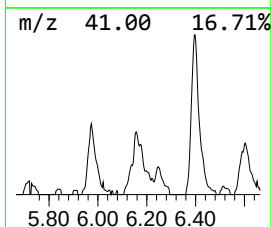
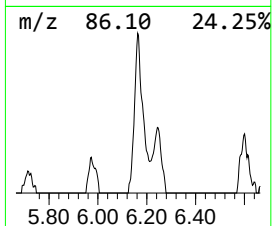
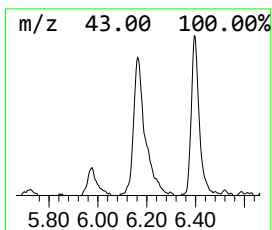
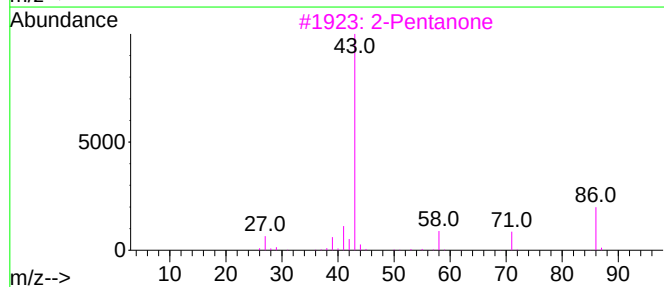
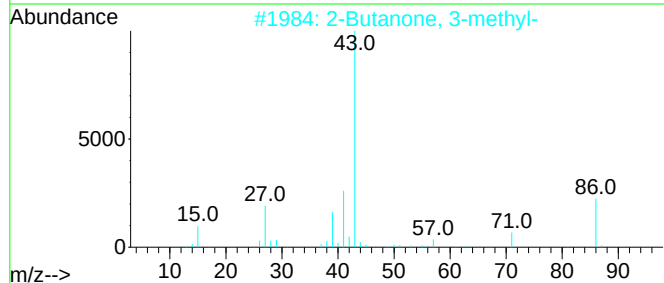
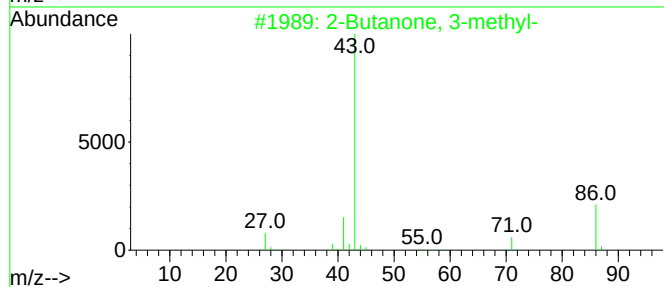
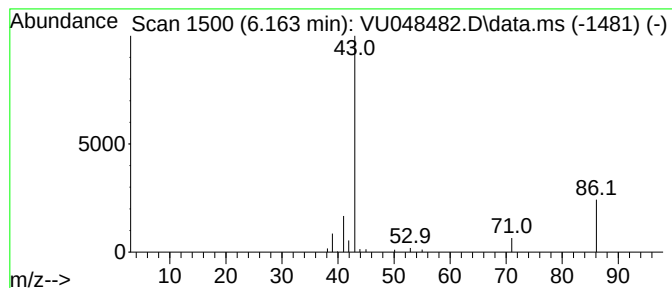
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Quant Title : VOC Analysis

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

Peak Number 4 2-Butanone, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.163	3.01 ug/L	54845	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3-methyl-			86	C5H10O	000563-80-4	64
2	2-Butanone, 3-methyl-			86	C5H10O	000563-80-4	43
3	2-Pentanone			86	C5H10O	000107-87-9	39
4	2-Pentanone			86	C5H10O	000107-87-9	38
5	2-Pentanone			86	C5H10O	000107-87-9	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051022\
Data File : VU048482.D
Acq On : 10 May 2022 11:44
Operator : SY/MD
Sample : N2708-07ME
Misc : 4.78g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL33ME

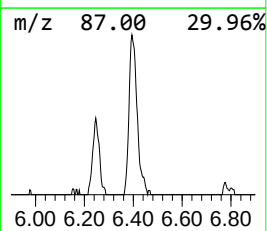
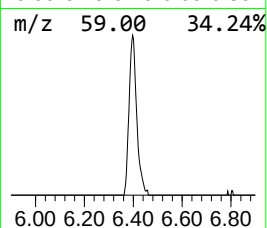
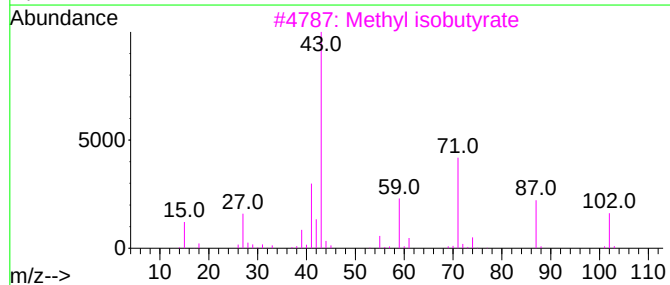
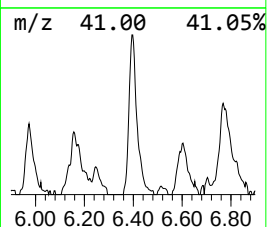
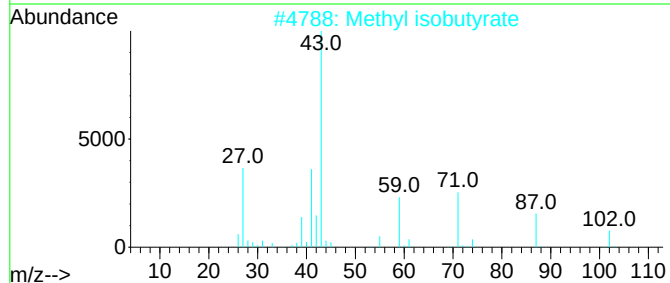
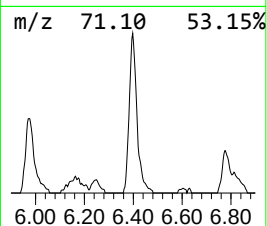
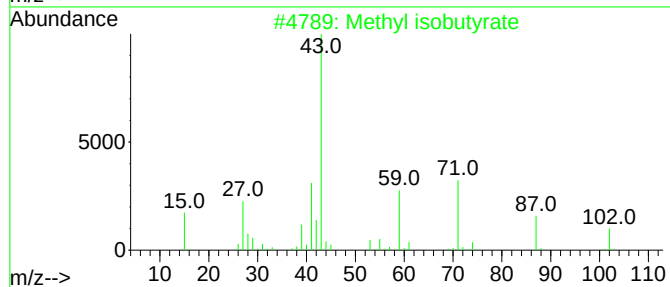
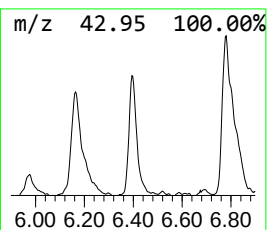
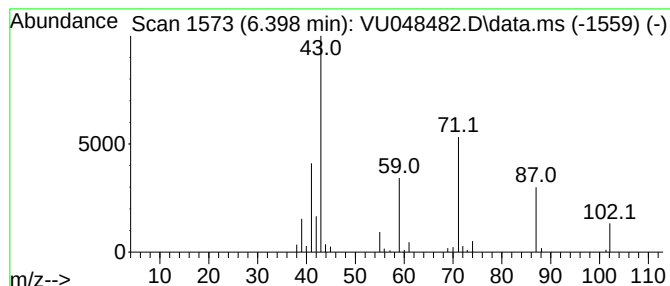
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Quant Title : VOC Analysis

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

Peak Number 5 Methyl isobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.398	5.36 ug/L	97714	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl isobutyrate	102	C5H10O2	000547-63-7	91
2			Methyl isobutyrate	102	C5H10O2	000547-63-7	83
3			Methyl isobutyrate	102	C5H10O2	000547-63-7	80
4			Methyl isobutyrate	102	C5H10O2	000547-63-7	64
5			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051022\
Data File : VU048482.D
Acq On : 10 May 2022 11:44
Operator : SY/MD
Sample : N2708-07ME
Misc : 4.78g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL33ME

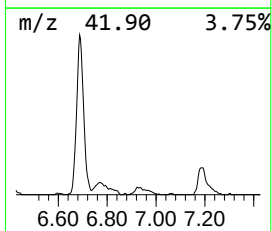
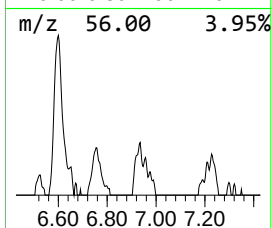
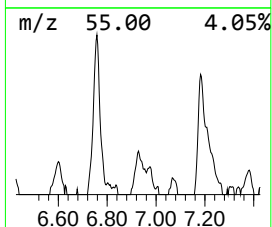
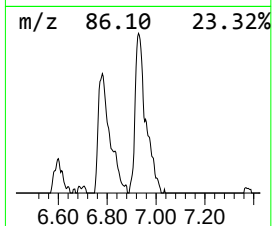
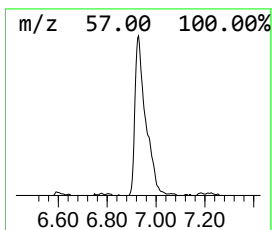
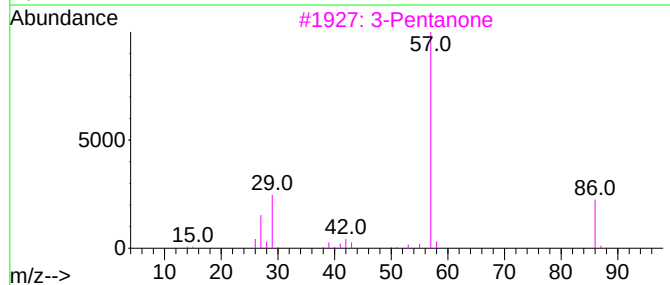
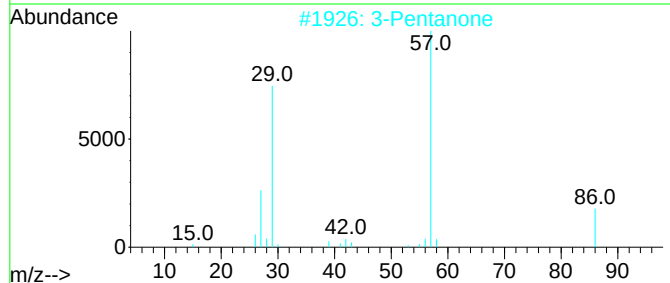
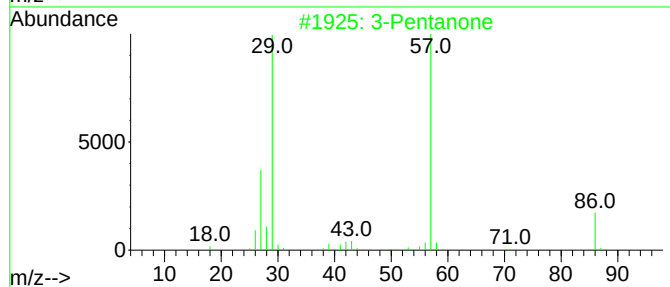
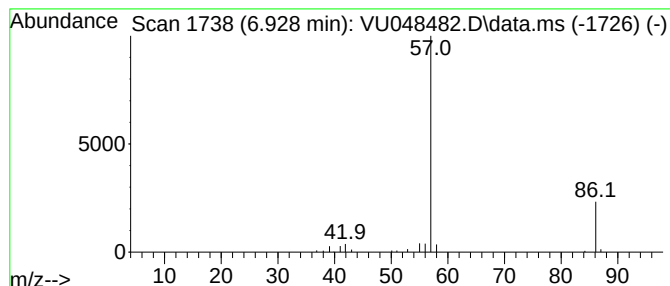
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Quant Title : VOC Analysis

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

Peak Number 6 3-Pentanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.928	5.07 ug/L	92511	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone			86	C5H10O	000096-22-0	86
2	3-Pentanone			86	C5H10O	000096-22-0	80
3	3-Pentanone			86	C5H10O	000096-22-0	64
4	3-Pentanone			86	C5H10O	000096-22-0	59
5	Propanal, 2,2-dimethyl-			86	C5H10O	000630-19-3	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051022\
Data File : VU048482.D
Acq On : 10 May 2022 11:44
Operator : SY/MD
Sample : N2708-07ME
Misc : 4.78g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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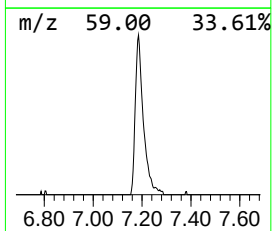
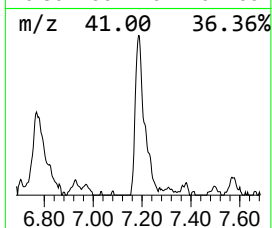
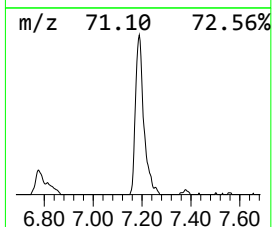
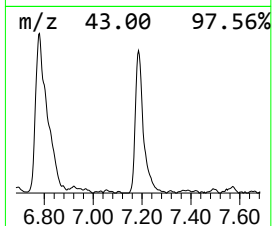
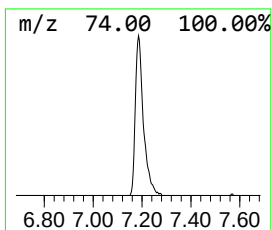
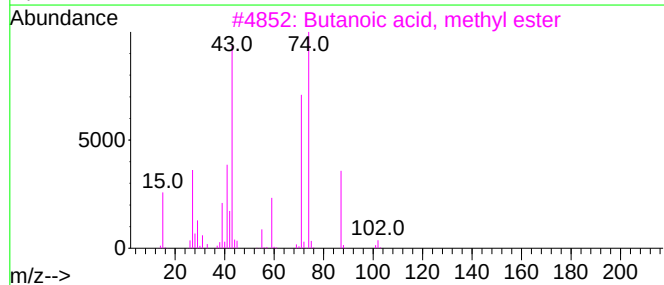
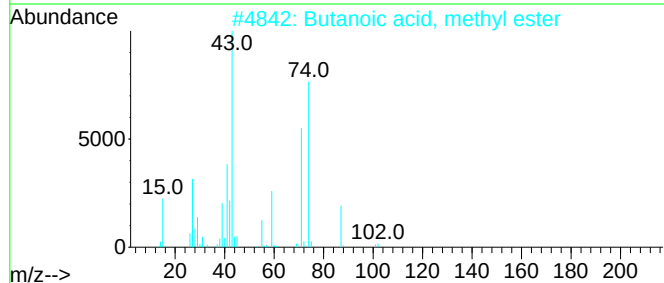
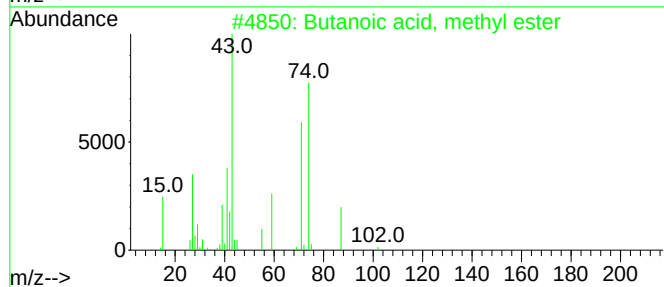
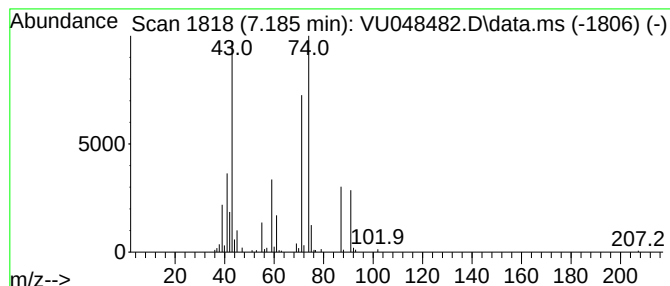
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Quant Title : VOC Analysis

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

Peak Number 7 Butanoic acid, methyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.185	11.46 ug/L	208882	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	87
2			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	83
3			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	72
4			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	64
5			Methyl isobutyrate	102	C5H10O2	000547-63-7	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051022\
Data File : VU048482.D
Acq On : 10 May 2022 11:44
Operator : SY/MD
Sample : N2708-07ME
Misc : 4.78g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL33ME

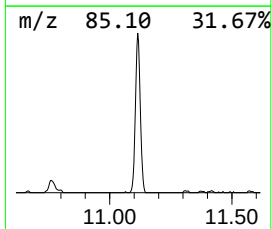
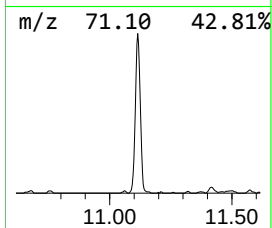
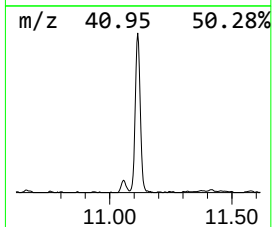
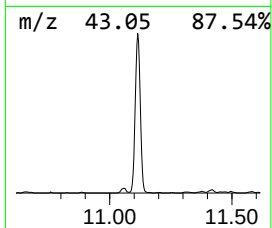
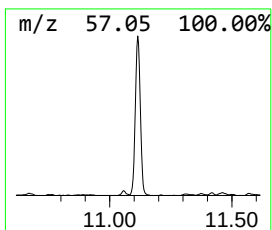
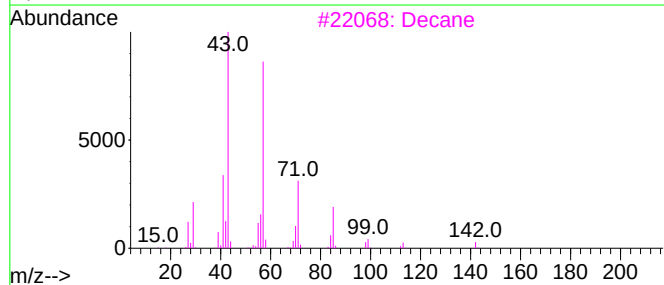
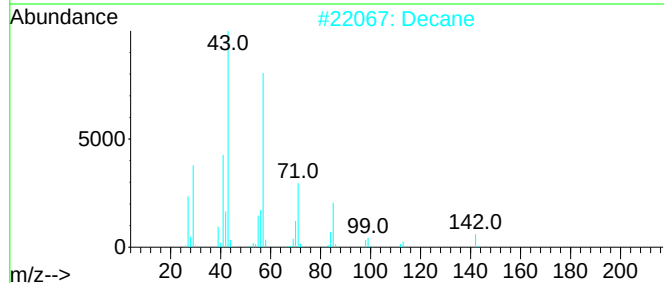
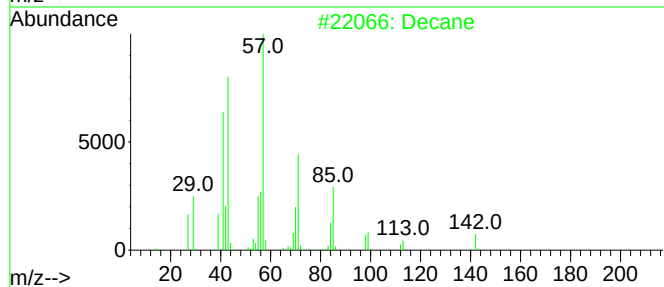
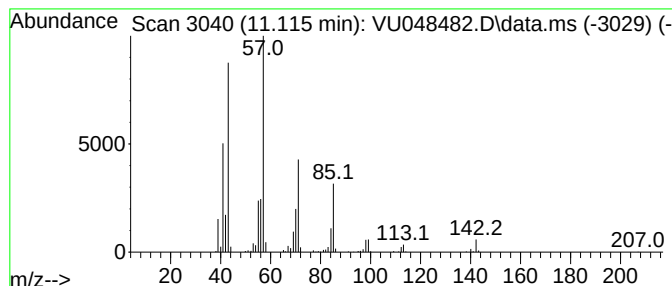
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Quant Title : VOC Analysis

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

Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.115	18.17 ug/L	422372	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane	142	C10H22	000124-18-5	96
2			Decane	142	C10H22	000124-18-5	91
3			Decane	142	C10H22	000124-18-5	90
4			Nonane	128	C9H20	000111-84-2	86
5			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051022\
Data File : VU048482.D
Acq On : 10 May 2022 11:44
Operator : SY/MD
Sample : N2708-07ME
Misc : 4.78g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL33ME

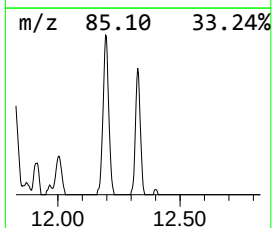
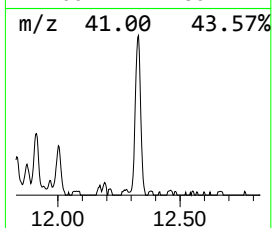
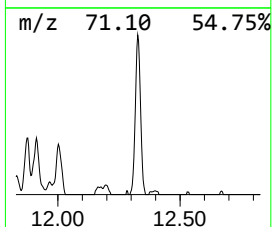
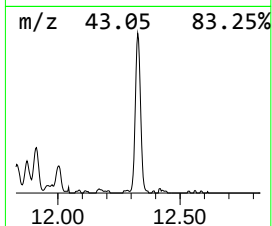
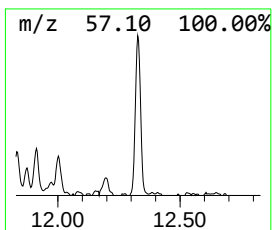
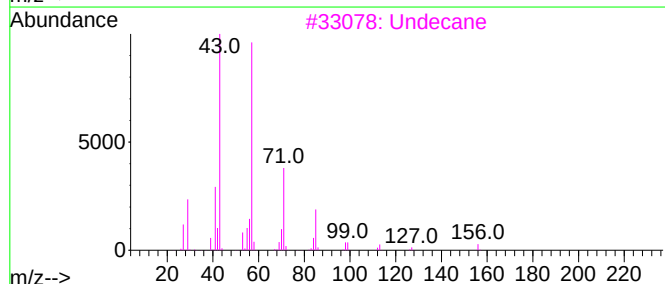
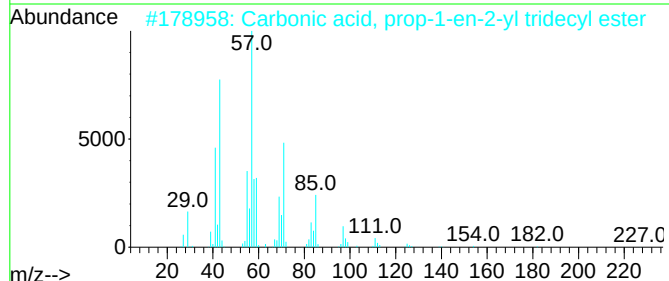
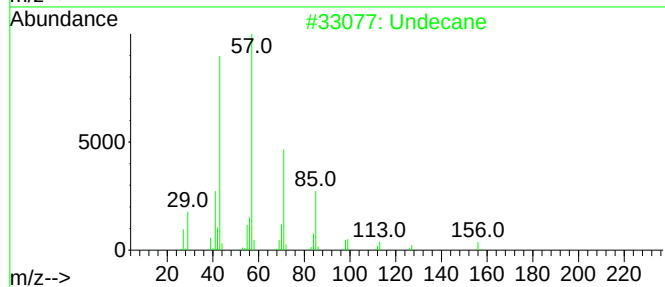
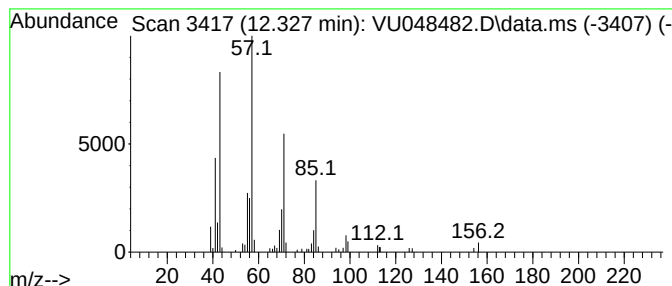
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Quant Title : VOC Analysis

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

Peak Number 10 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.327	4.05 ug/L	94060	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane	156	C11H24	001120-21-4	87
2			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	86
3			Undecane	156	C11H24	001120-21-4	81
4			Undecane	156	C11H24	001120-21-4	74
5			Undecane	156	C11H24	001120-21-4	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051022\
Data File : VU048482.D
Acq On : 10 May 2022 11:44
Operator : SY/MD
Sample : N2708-07ME
Misc : 4.78g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL33ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.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
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Methyl propionate	5.195	6.4	ug/L	116796	1	6.247	911746	50.0
2-Butanone, 3-m...	6.163	3.0	ug/L	54845	1	6.247	911746	50.0
Methyl isobutyrate	6.398	5.4	ug/L	97714	1	6.247	911746	50.0
3-Pentanone	6.928	5.1	ug/L	92511	1	6.247	911746	50.0
Butanoic acid, ...	7.185	11.5	ug/L	208882	1	6.247	911746	50.0
(DEL) Alkane: S...	11.115	18.2	ug/L	422372	3	11.816	1162460	50.0
(DEL) Alkane: S...	12.327	4.0	ug/L	94060	3	11.816	1162460	50.0