

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052522\
 Data File : VU048664.D
 Acq On : 25 May 2022 12:30
 Operator : SY/MD
 Sample : N2925-09ME
 Misc : 4.94g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXXY6ME

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\SFAMULM051622WMA.M
 Title : VOC Analysis

Signal : TIC: VU048664.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	37	43	65	rVB	80282	95774	11.51%	1.319%
2	1.594	73	79	87	rBV	27881	37937	4.56%	0.523%
3	1.777	130	136	137	rBV3	1906	1866	0.22%	0.026%
4	2.205	266	269	270	rBV2	308	181	0.02%	0.002%
5	2.321	295	305	307	rBV2	2846	3154	0.38%	0.043%
6	2.536	363	372	385	rVB	197387	314297	37.76%	4.329%
7	3.562	688	691	692	rBV2	825	423	0.05%	0.006%
8	3.642	713	716	718	rBV2	397	240	0.03%	0.003%
9	3.710	735	737	738	rBV	387	150	0.02%	0.002%
10	3.793	758	763	766	rBV	471	425	0.05%	0.006%
11	3.890	790	793	795	rBV	449	315	0.04%	0.004%
12	3.964	813	816	817	rBV	351	219	0.03%	0.003%
13	4.112	858	862	865	rBV	560	592	0.07%	0.008%
14	4.147	870	873	876	rBV	500	382	0.05%	0.005%
15	4.289	915	917	919	rBV	290	149	0.02%	0.002%
16	4.324	925	928	931	rBV	415	344	0.04%	0.005%
17	4.379	941	945	948	rVB	496	322	0.04%	0.004%
18	4.398	948	951	954	rBV	446	305	0.04%	0.004%
19	4.488	976	979	981	rBV	397	255	0.03%	0.004%
20	4.639	1013	1026	1038	rBV2	51832	151816	18.24%	2.091%
21	5.063	1141	1158	1188	rBV	147581	357012	42.89%	4.917%
22	5.202	1191	1201	1219	rVV	24704	54538	6.55%	0.751%
23	5.719	1341	1362	1386	rBV2	257026	684162	82.20%	9.424%
24	5.874	1401	1410	1411	rBV	961	1224	0.15%	0.017%
25	5.973	1431	1441	1455	rBV6	7055	17581	2.11%	0.242%
26	6.166	1491	1501	1513	rBV5	8511	21675	2.60%	0.299%
27	6.247	1514	1526	1549	rVB	280592	560479	67.34%	7.720%
28	6.398	1562	1573	1590	rBV2	23836	52624	6.32%	0.725%
29	6.530	1603	1614	1622	rBV6	5056	9134	1.10%	0.126%
30	6.690	1651	1664	1681	rBV2	150156	308795	37.10%	4.253%
31	6.932	1730	1739	1752	rBV	15396	38644	4.64%	0.532%
32	7.189	1808	1819	1846	rBV3	43291	109972	13.21%	1.515%
33	7.369	1870	1875	1876	rBV	914	757	0.09%	0.010%
34	7.526	1921	1924	1925	rBV	287	159	0.02%	0.002%
35	7.568	1925	1937	1955	rVV	87260	171101	20.56%	2.357%
36	7.732	1986	1988	1989	rBV	376	168	0.02%	0.002%

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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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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\SFAMULM051622WMA.M
 Title : VOC Analysis

37	7.793	1999	2007	2018	rBV5	2413	4544	0.55%	0.063%
38	7.899	2026	2040	2056	rBV	296051	539275	64.79%	7.428%
39	8.182	2116	2128	2150	rBV2	74519	173825	20.88%	2.394%
40	8.420	2198	2202	2206	rBV3	873	750	0.09%	0.010%
41	8.665	2260	2278	2296	rBV	184771	436090	52.39%	6.007%
42	8.861	2338	2339	2341	rBV2	439	175	0.02%	0.002%
43	9.240	2454	2457	2459	rBV	427	280	0.03%	0.004%
44	9.423	2500	2514	2533	rBV	347997	690715	82.98%	9.514%
45	9.610	2569	2572	2575	rVB3	561	388	0.05%	0.005%
46	9.636	2575	2580	2586	rBV	563	728	0.09%	0.010%
47	9.700	2588	2600	2608	rVV5	4519	8250	0.99%	0.114%
48	9.835	2637	2642	2645	rBV	937	740	0.09%	0.010%
49	9.861	2645	2650	2653	rVV	470	451	0.05%	0.006%
50	10.044	2704	2707	2712	rBV2	574	618	0.07%	0.009%
51	10.382	2809	2812	2814	rBV	546	331	0.04%	0.005%
52	10.767	2919	2932	2948	rVB2	280823	466883	56.09%	6.431%
53	10.964	2991	2993	2994	rBV2	344	137	0.02%	0.002%
54	11.060	3014	3023	3030	rBV4	17320	25796	3.10%	0.355%
55	11.118	3031	3041	3055	rVB	228975	334631	40.20%	4.609%
56	11.578	3178	3184	3187	rBV5	1555	1994	0.24%	0.027%
57	11.819	3247	3259	3272	rBV	515945	832356	100.00%	11.465%
58	12.147	3358	3361	3363	rBV2	392	294	0.04%	0.004%
59	12.198	3364	3377	3404	rVB	413717	663171	79.67%	9.135%
60	12.330	3409	3418	3428	rVB2	32006	46455	5.58%	0.640%
61	13.176	3677	3681	3682	rBV	588	456	0.05%	0.006%
62	13.391	3741	3748	3756	rBV4	17013	21985	2.64%	0.303%
63	13.703	3838	3845	3848	rBV2	1053	1307	0.16%	0.018%
64	14.092	3959	3966	3974	rBV	7390	10272	1.23%	0.141%

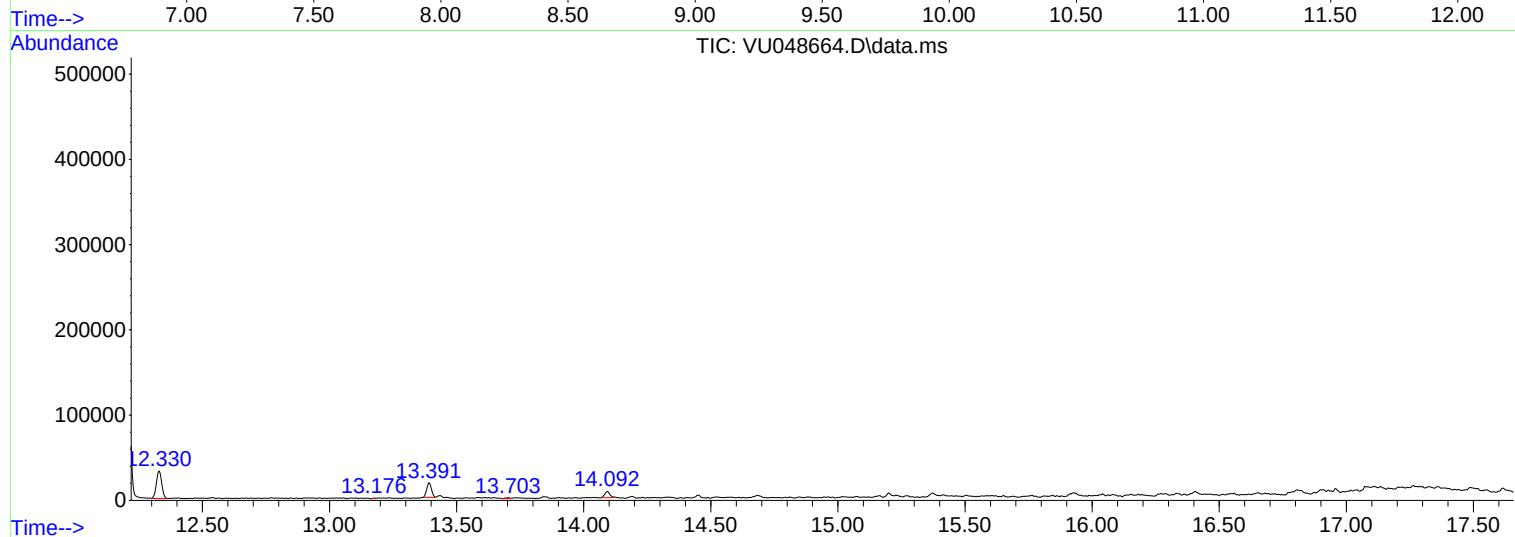
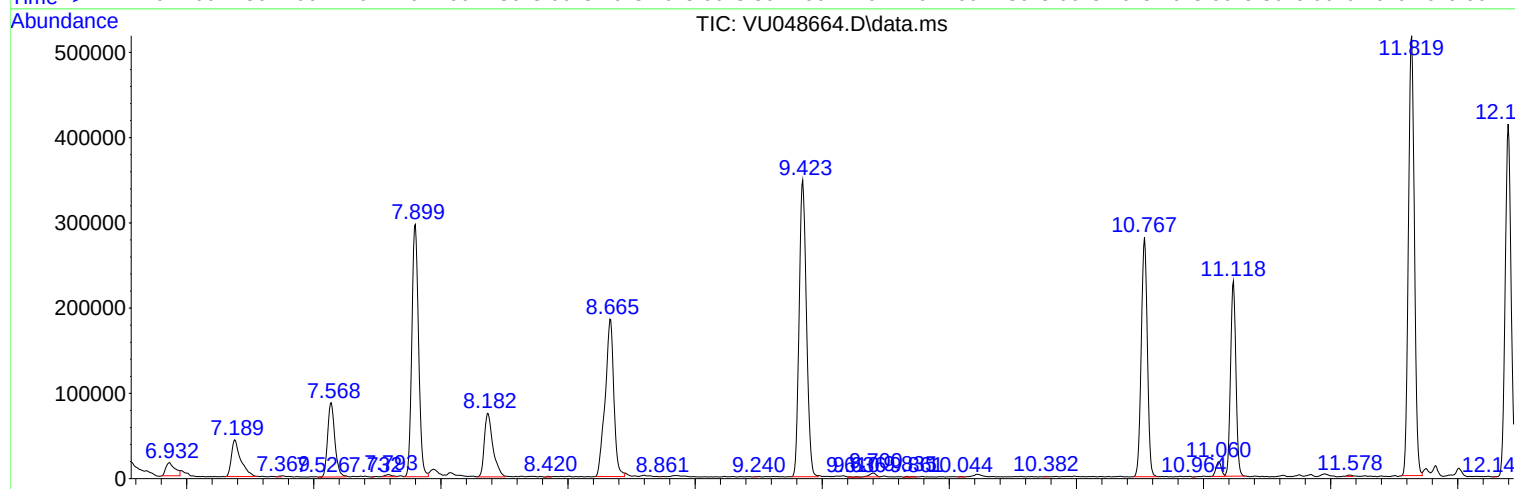
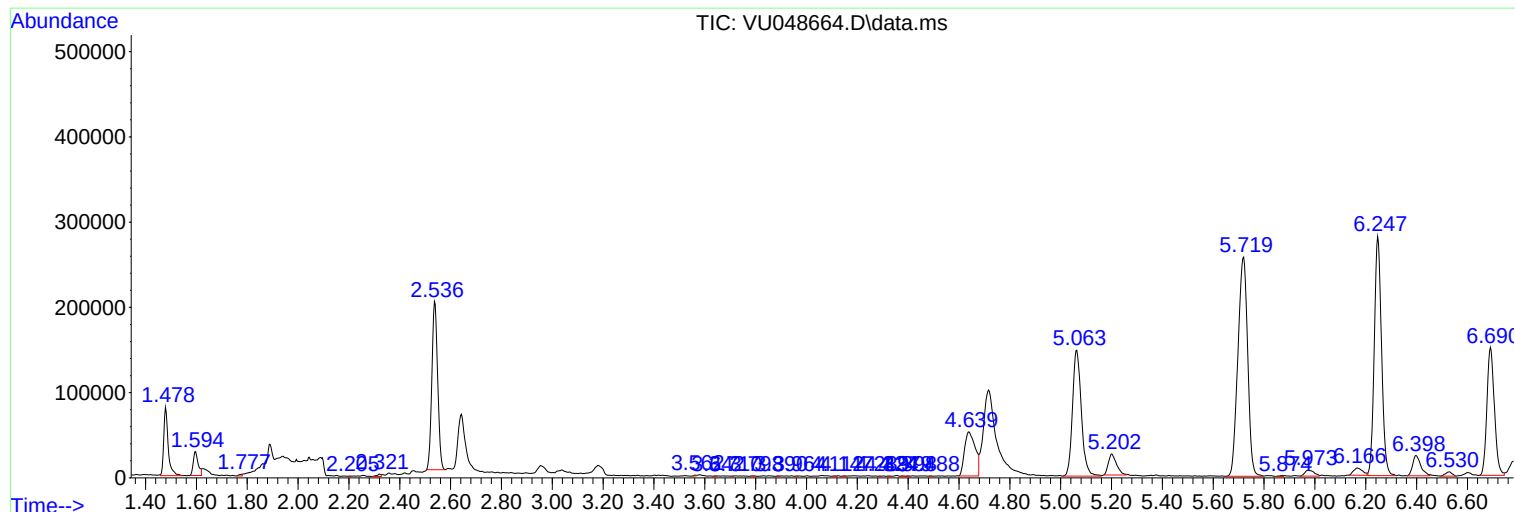
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Instrument :
MSVOA_U
ClientSampleId :
EXXY6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXXY6ME

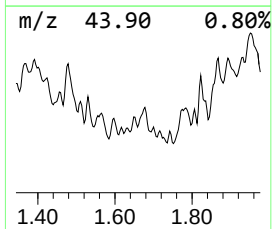
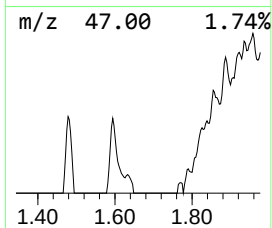
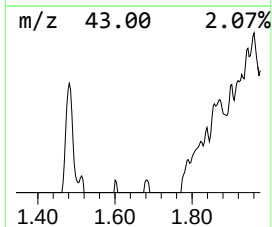
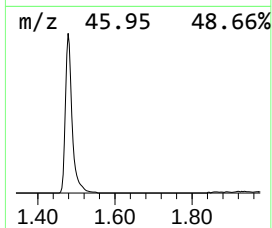
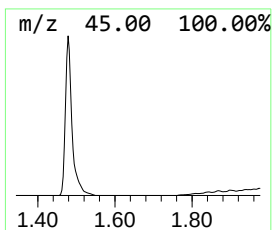
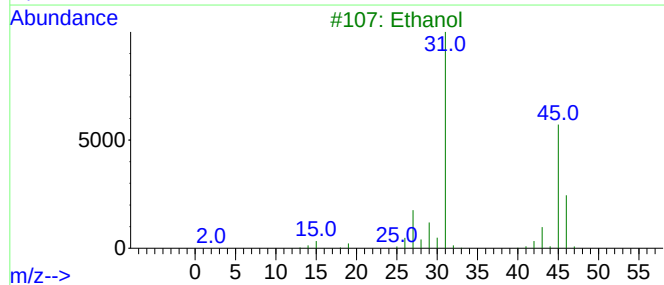
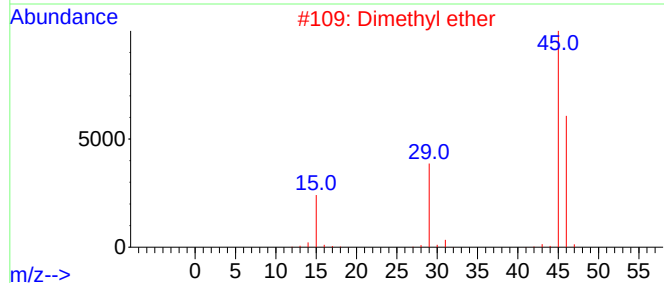
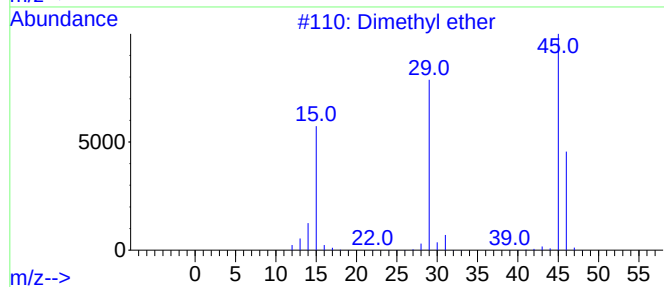
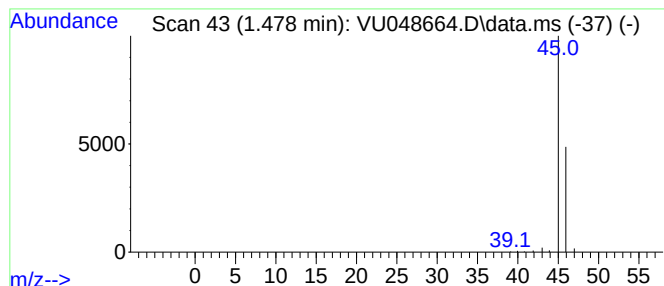
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Quant Title : VOC Analysis

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

Peak Number 1 Dimethyl ether Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.478	8.54 ug/L	95774	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl ether	46	C2H6O	000115-10-6	90
2			Dimethyl ether	46	C2H6O	000115-10-6	74
3			Ethanol	46	C2H6O	000064-17-5	7
4			Ethanol	46	C2H6O	000064-17-5	7
5			Ethanol	46	C2H6O	000064-17-5	7



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ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXXY6ME

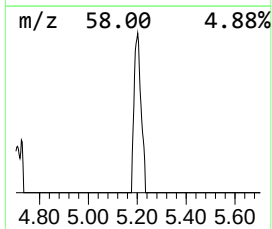
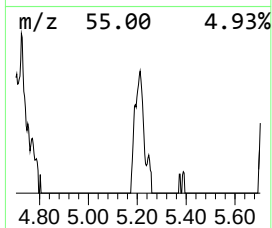
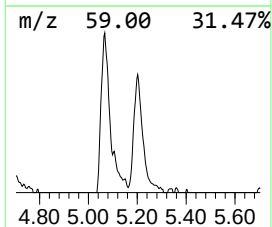
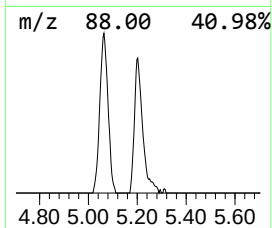
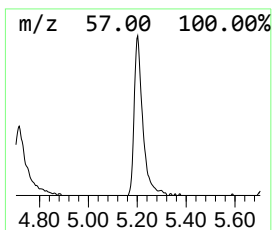
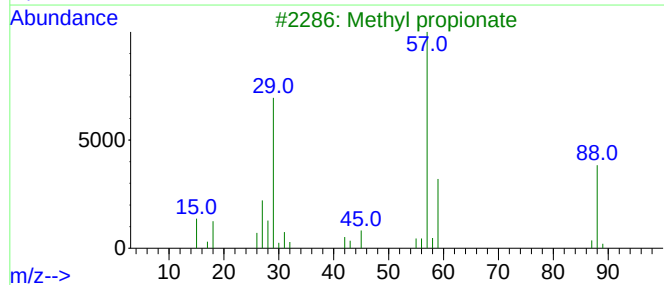
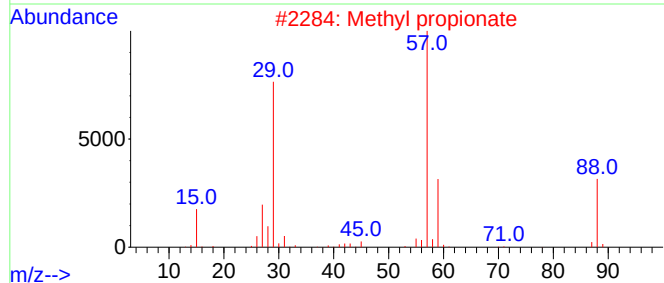
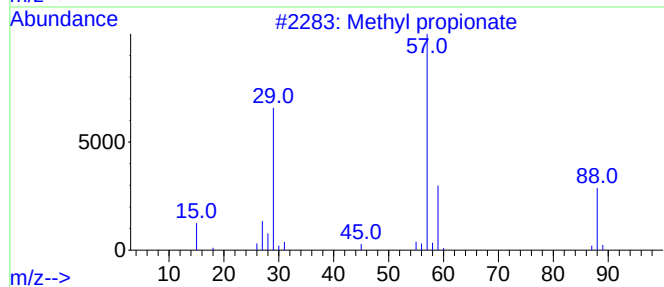
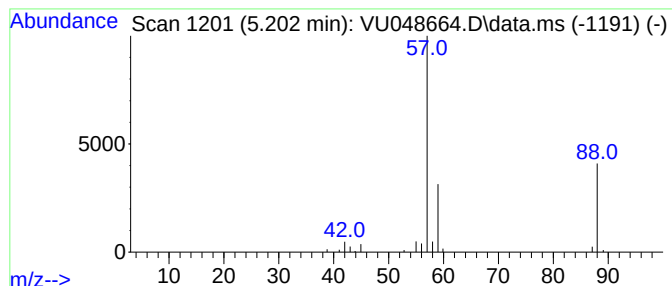
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Methyl propionate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.202	4.87 ug/L	54538	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	80
3	Methyl propionate			88	C4H8O2	000554-12-1	78
4	Methyl propionate			88	C4H8O2	000554-12-1	78
5	Methyl propionate			88	C4H8O2	000554-12-1	72



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Operator : SY/MD
Sample : N2925-09ME
Misc : 4.94g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXXY6ME

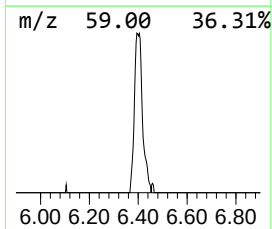
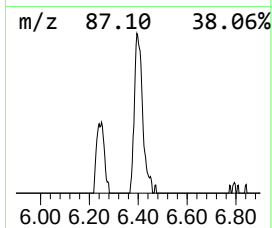
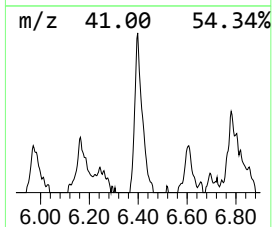
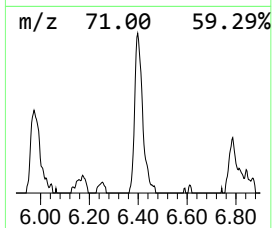
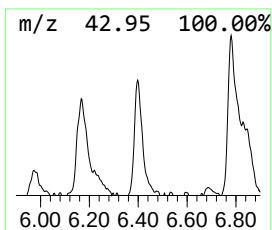
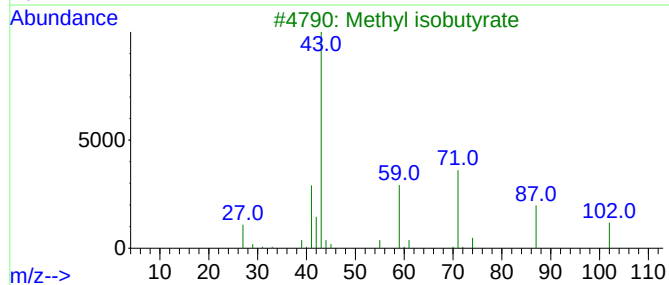
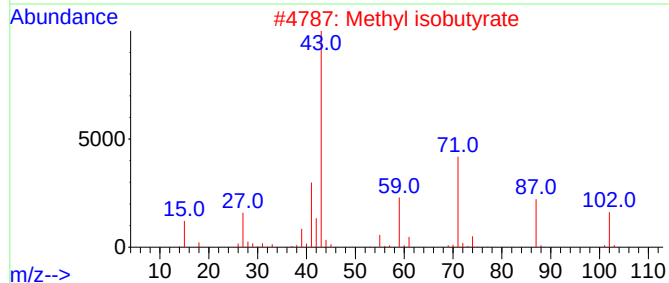
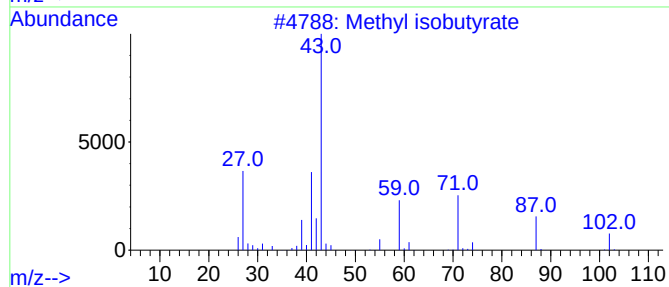
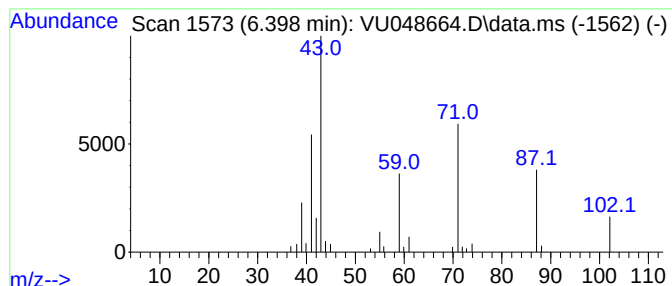
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Methyl isobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.398	4.69 ug/L	52624	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl isobutyrate	102	C5H10O2	000547-63-7	87
2			Methyl isobutyrate	102	C5H10O2	000547-63-7	86
3			Methyl isobutyrate	102	C5H10O2	000547-63-7	52
4			Methyl isobutyrate	102	C5H10O2	000547-63-7	46
5			Butyric acid hydrazide	102	C4H10N2O	003538-65-6	43



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Instrument :
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EXXY6ME

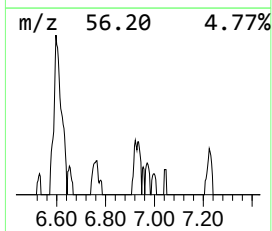
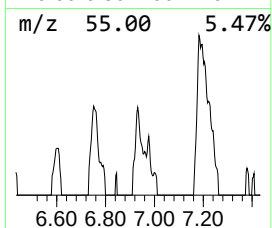
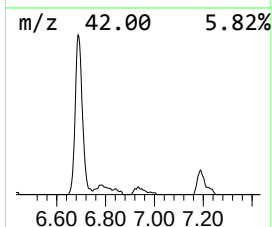
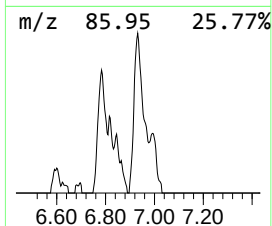
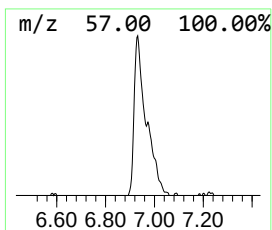
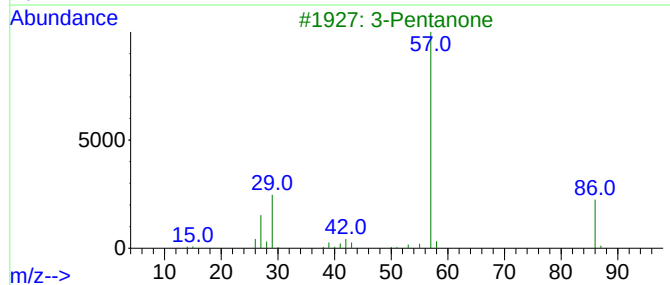
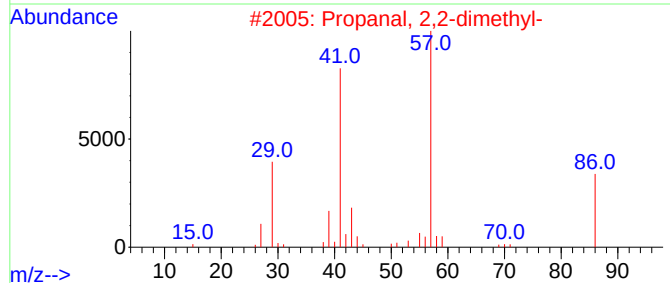
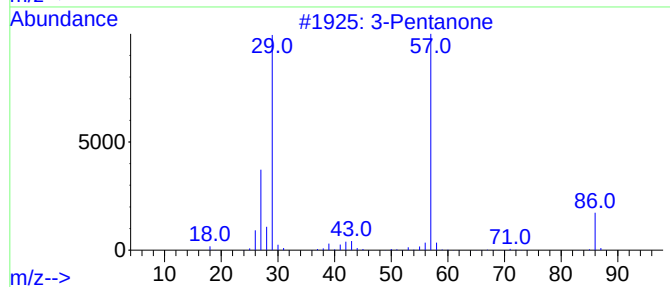
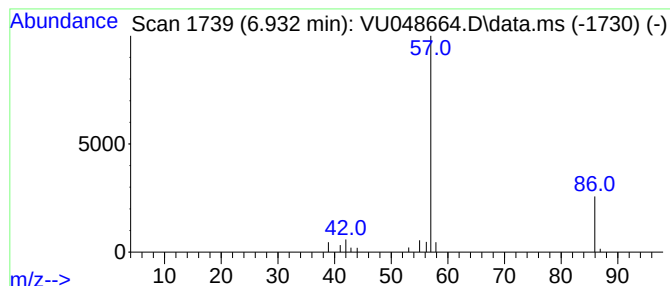
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 3-Pentanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.932	3.45 ug/L	38644	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone			86	C5H10O	000096-22-0	86
2	Propanal, 2,2-dimethyl-			86	C5H10O	000630-19-3	80
3	3-Pentanone			86	C5H10O	000096-22-0	72
4	3-Pentanone			86	C5H10O	000096-22-0	72
5	3-Pentanone			86	C5H10O	000096-22-0	28



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ClientSampleId :
EXXY6ME

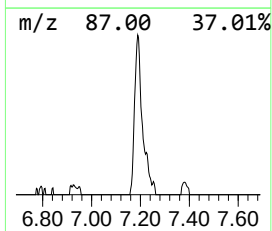
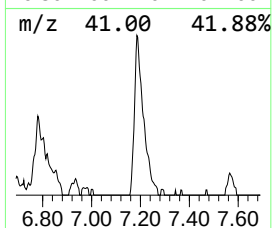
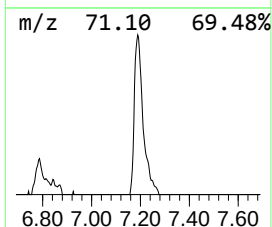
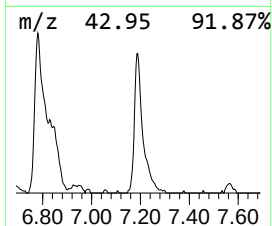
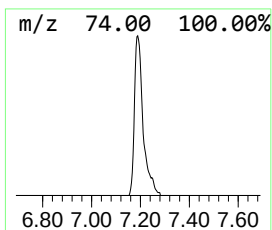
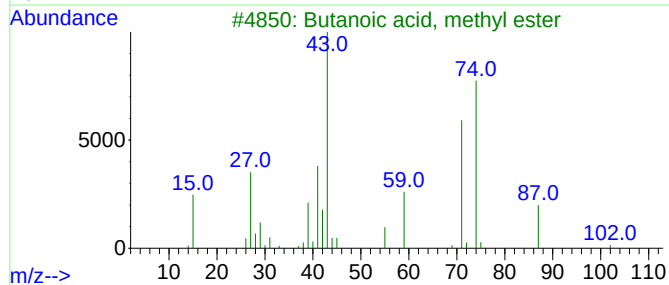
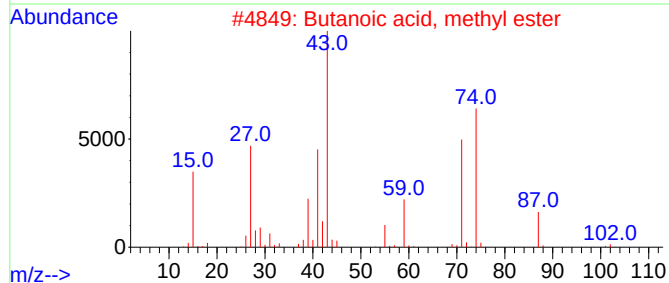
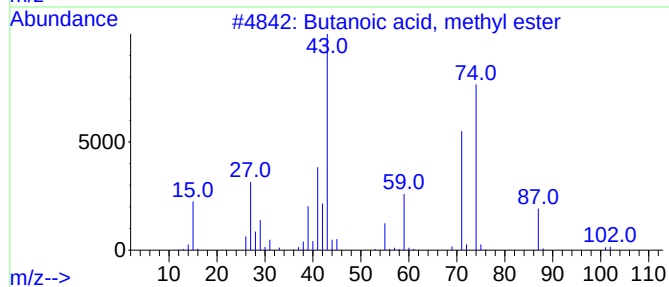
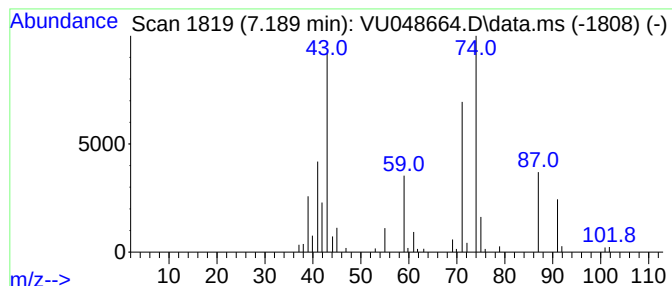
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Quant Title : VOC Analysis

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

Peak Number 5 Butanoic acid, methyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.189	9.81 ug/L	109972	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	81
2			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	80
3			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	74
4			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	56
5			Hexanoic acid, methyl ester	130	C7H14O2	000106-70-7	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052522\
Data File : VU048664.D
Acq On : 25 May 2022 12:30
Operator : SY/MD
Sample : N2925-09ME
Misc : 4.94g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXXY6ME

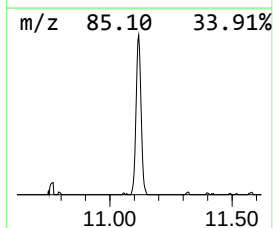
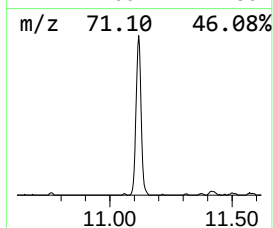
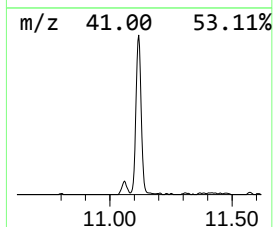
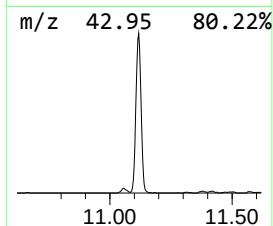
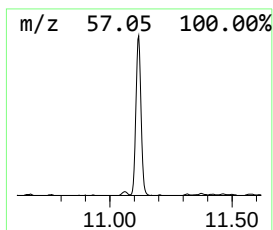
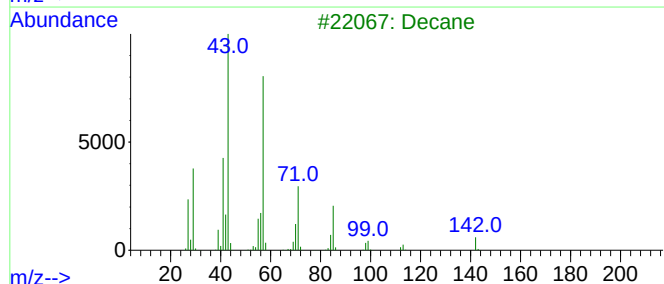
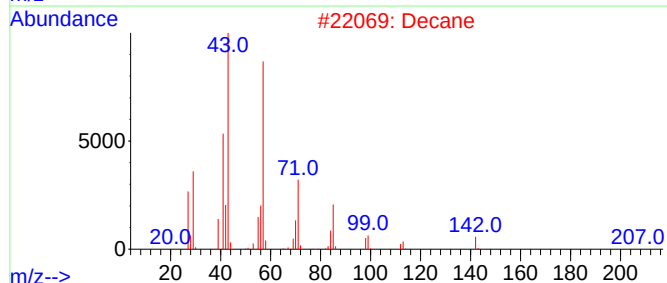
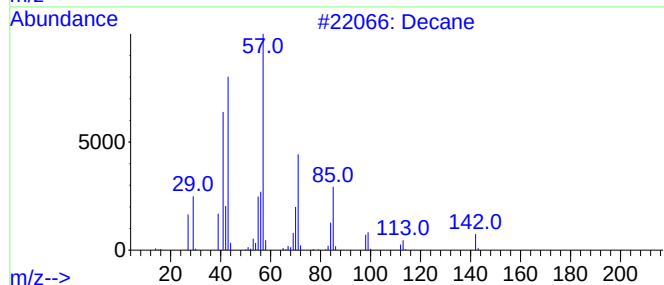
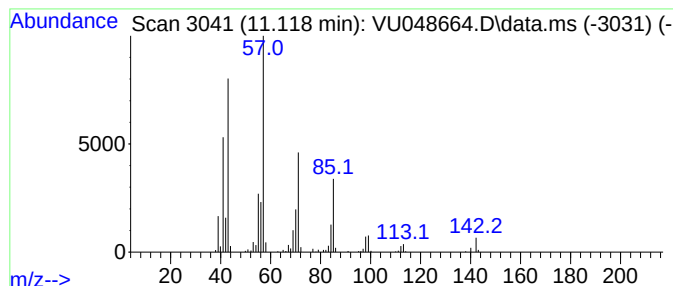
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Quant Title : VOC Analysis

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.118	20.10 ug/L	334631	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane	142	C10H22	000124-18-5	96
2			Decane	142	C10H22	000124-18-5	95
3			Decane	142	C10H22	000124-18-5	95
4			Decane	142	C10H22	000124-18-5	91
5			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052522\
Data File : VU048664.D
Acq On : 25 May 2022 12:30
Operator : SY/MD
Sample : N2925-09ME
Misc : 4.94g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXXY6ME

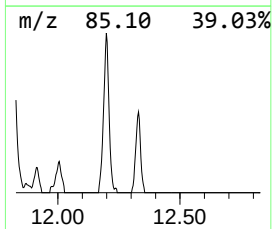
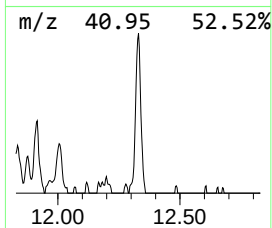
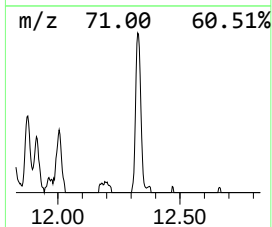
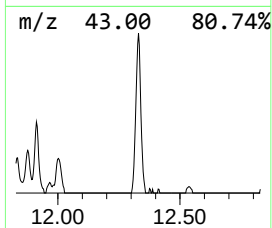
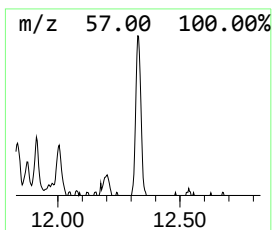
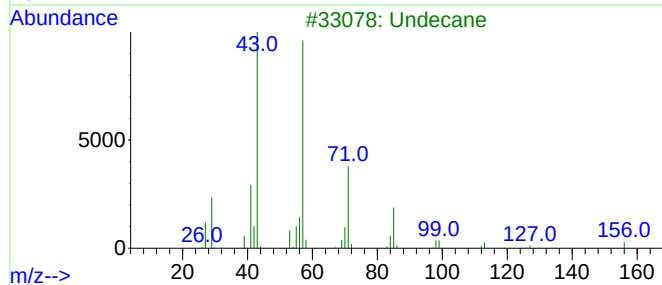
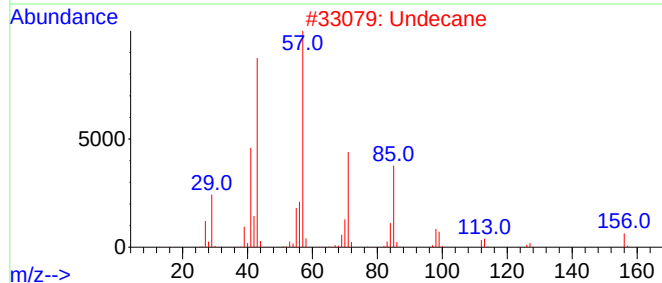
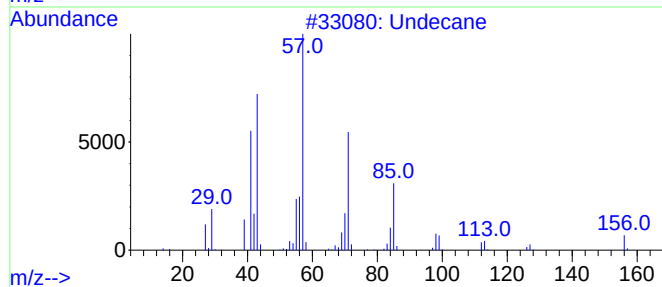
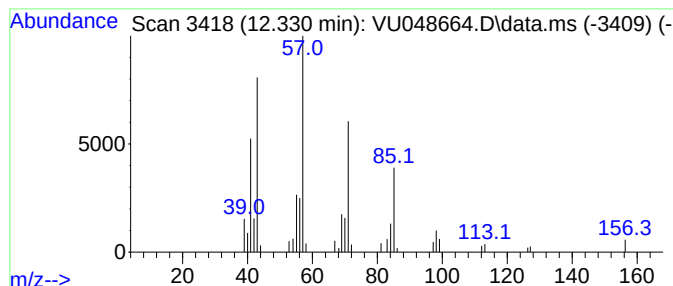
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

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.
12.330	2.79 ug/L	46455	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	94
2	Undecane			156	C11H24	001120-21-4	93
3	Undecane			156	C11H24	001120-21-4	87
4	Tetradecane			198	C14H30	000629-59-4	78
5	Undecane			156	C11H24	001120-21-4	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052522\
Data File : VU048664.D
Acq On : 25 May 2022 12:30
Operator : SY/MD
Sample : N2925-09ME
Misc : 4.94g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXXY6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.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
Dimethyl ether	1.478	8.5	ug/L	95774	1	6.247	560479	50.0
Methyl propionate	5.202	4.9	ug/L	54538	1	6.247	560479	50.0
Methyl isobutyrate	6.398	4.7	ug/L	52624	1	6.247	560479	50.0
3-Pentanone	6.932	3.5	ug/L	38644	1	6.247	560479	50.0
Butanoic acid, ...	7.189	9.8	ug/L	109972	1	6.247	560479	50.0
(DEL) Alkane: S...	11.118	20.1	ug/L	334631	3	11.819	832356	50.0
(DEL) Alkane: S...	12.330	2.8	ug/L	46455	3	11.819	832356	50.0