LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052522\
Data File : VU048666.D
Acq On : 25 May 2022 13:19
Operator : SY/MD
Sample : N2926-13ME
Misc : 3.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY23ME

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: VU048666.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	59	rVB	78239	95695	11.49%	1.314%
2	1.594	73	79	99	rBV	33726	55477	6.66%	0.762%
3	2.122	238	243	245	rBV2	415	382	0.05%	0.005%
4	2.231	273	277	280	rVB	521	374	0.04%	0.005%
5	2.298	294	298	300	rVB2	272	201	0.02%	0.003%
6	2.334	305	309	311	rBV2	330	269	0.03%	0.004%
7	2.359	314	317	320	rBV4	572	350	0.04%	0.005%
8	2.536	360	372	384	rBV	114216	184281	22.13%	2.530%
9	2.636	395	403	422	rVB2	25966	49609	5.96%	0.681%
10	2.794	449	452	454	rBV2	480	306	0.04%	0.004%
11	2.851	467	470	475	rBV2	518	475	0.06%	0.007%
12	2.951	492	501	512	rBV3	9764	18811	2.26%	0.258%
13	3.125	551	555	558	rBV	450	366	0.04%	0.005%
14	3.179	558	572	588	rBV	14112	35536	4.27%	0.488%
15	3.543	683	685	689	rBV	358	307	0.04%	0.004%
16	3.568	689	693	695	rBV3	1031	963	0.12%	0.013%
17	3.626	705	711	721	rBV2	833	1698	0.20%	0.023%
18	3.716	736	739	741	rBV	398	263	0.03%	0.004%
19	3.912	794	800	801	rBV	507	493	0.06%	0.007%
20	4.263	906	909	913	rBV	517	375	0.05%	0.005%
21	4.359	936	939	942	rBV	570	401	0.05%	0.006%
22	4.552	996	999	1002	rBV	475	408	0.05%	0.006%
23	4.633	1010	1024	1037	rBV	64305	178801	21.47%	2.454%
24	4.999	1133	1138	1140	rBV	726	603	0.07%	0.008%
25	5.060	1142	1157	1180	rVB2	153822	352079	42.28%	4.833%
26	5.195	1189	1199	1212	rBV3	25449	54959	6.60%	0.754%
27	5.472	1281	1285	1288	rBV	487	422	0.05%	0.006%
28	5.617	1327	1330	1332	rBV	342	256	0.03%	0.004%
29	5.716	1341	1361	1386	rBV2	256181	683399	82.08%	9.381%
30	5.935	1427	1429	1430	rBV	423	208	0.02%	0.003%
31	5.970	1431	1440	1462	rVV6	7120	17525	2.10%	0.241%
32	6.047	1462	1464	1471	rVB2	607	477	0.06%	0.007%
33	6.160	1486	1499	1512	rBV4	8747	24021	2.88%	0.330%
34	6.247	1513	1526	1551	rVB	270217	539531	64.80%	7.406%
35	6.395	1561	1572	1596	rVB3	23253	52810	6.34%	0.725%
36	6.527	1602	1613	1625	rBV6	4513	8951	1.08%	0.123%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052522\
Data File : VU048666.D
Acq On : 25 May 2022 13:19
Operator : SY/MD
Sample : N2926-13ME
Misc : 3.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY23ME

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

37	6.591	1625	1633	1644	rBV6	3852	7654	0.92%	0.105%
38	6.690	1650	1664	1681	rBV	150605	308700	37.07%	4.237%
39	6.925	1727	1737	1749	rBV2	17155	42733	5.13%	0.587%
40	7.035	1769	1771	1777	rVB2	675	596	0.07%	0.008%
41	7.063	1777	1780	1781	rBV	823	444	0.05%	0.006%
42	7.186	1806	1818	1840	rBV3	43791	103243	12.40%	1.417%
43	7.311	1854	1857	1861	rBV3	471	421	0.05%	0.006%
44	7.372	1871	1876	1879	rBV2	1289	1359	0.16%	0.019%
45	7.433	1892	1895	1898	rBV	424	270	0.03%	0.004%
46	7.475	1905	1908	1914	rVB	549	445	0.05%	0.006%
47	7.507	1914	1918	1921	rBV	677	643	0.08%	0.009%
48	7.565	1925	1936	1958	rVB2	89963	173067	20.79%	2.376%
49	7.645	1958	1961	1965	rBV	359	255	0.03%	0.004%
50	7.687	1970	1974	1981	rVV3	1244	1429	0.17%	0.020%
51	7.790	1997	2006	2008	rBV5	2518	3635	0.44%	0.050%
52	7.896	2026	2039	2055	rBV	297556	535608	64.33%	7.352%
53	8.182	2117	2128	2148	rBV4	79747	168168	20.20%	2.308%
54	8.311	2164	2168	2173	rVB3	949	903	0.11%	0.012%
55	8.337	2173	2176	2178	rBV	656	391	0.05%	0.005%
56	8.366	2181	2185	2187	rBV4	566	441	0.05%	0.006%
57	8.420	2199	2202	2204	rBV	382	209	0.03%	0.003%
58	8.436	2204	2207	2208	rBV	382	235	0.03%	0.003%
59	8.555	2234	2244	2252	rVB5	10570	18153	2.18%	0.249%
60	8.652	2258	2274	2308	rBV	206703	474864	57.03%	6.518%
61	8.906	2350	2353	2355	rBV	430	278	0.03%	0.004%
62	8.925	2355	2359	2363	rVV5	930	1080	0.13%	0.015%
63	9.002	2380	2383	2387	rVB2	542	440	0.05%	0.006%
64	9.173	2434	2436	2438	rBV	377	210	0.03%	0.003%
65	9.305	2474	2477	2482	rBV	687	532	0.06%	0.007%
66	9.330	2482	2485	2487	rBV	489	306	0.04%	0.004%
67	9.420	2500	2513	2532	rBV	366320	682647	81.98%	9.371%
68	9.559	2552	2556	2557	rBV2	845	474	0.06%	0.007%
69	9.616	2572	2574	2576	rBV	434	215	0.03%	0.003%
70	9.655	2581	2586	2588	rBV2	650	575	0.07%	0.008%
71	9.694	2592	2598	2609	rVB4	3084	5194	0.62%	0.071%
72	9.841	2640	2644	2647	rBV	494	367	0.04%	0.005%
73	9.960	2679	2681	2683	rBV	418	237	0.03%	0.003%
74	10.005	2691	2695	2698	rBV2	525	509	0.06%	0.007%
75	10.057	2707	2711	2713	rBV	408	272	0.03%	0.004%
76	10.112	2719	2728	2737	rBV6	2421	3896	0.47%	0.053%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052522\
Data File : VU048666.D
Acq On : 25 May 2022 13:19
Operator : SY/MD
Sample : N2926-13ME
Misc : 3.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY23ME

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

77	10.240	2765	2768	2770	rBV2	507	344	0.04%	0.005%
78	10.301	2780	2787	2793	rVB	848	1086	0.13%	0.015%
79	10.343	2793	2800	2802	rBV2	581	586	0.07%	0.008%
80	10.407	2816	2820	2829	rVB2	602	677	0.08%	0.009%
81	10.452	2829	2834	2838	rBV2	505	530	0.06%	0.007%
82	10.488	2839	2845	2847	rBV2	633	604	0.07%	0.008%
83	10.597	2875	2879	2883	rBV2	630	640	0.08%	0.009%
84	10.764	2918	2931	2948	rBV	289162	477948	57.40%	6.561%
85	10.896	2964	2972	2982	rVB3	4127	7337	0.88%	0.101%
86	11.057	3014	3022	3030	rBV4	15980	22526	2.71%	0.309%
87	11.115	3030	3040	3057	rVB	186391	277567	33.34%	3.810%
88	11.279	3088	3091	3093	rBV2	687	446	0.05%	0.006%
89	11.411	3128	3132	3135	rBV5	1805	1921	0.23%	0.026%
90	11.578	3174	3184	3189	rBV5	1952	2803	0.34%	0.038%
91	11.636	3198	3202	3203	rBV3	871	597	0.07%	0.008%
92	11.816	3246	3258	3271	rBV	519763	832651	100.00%	11.430%
93	12.195	3364	3376	3392	rBV	424782	675682	81.15%	9.275%
94	12.330	3409	3418	3427	rVB2	32237	45601	5.48%	0.626%
95	12.584	3493	3497	3500	rBV2	706	530	0.06%	0.007%
96	12.710	3531	3536	3538	rBV	480	452	0.05%	0.006%
97	13.391	3739	3748	3756	rBV4	19067	25965	3.12%	0.356%
98	13.922	3910	3913	3917	rBV2	726	575	0.07%	0.008%
99	14.452	4072	4078	4087	rVB5	4244	5244	0.63%	0.072%
100	14.632	4131	4134	4136	rBV2	794	570	0.07%	0.008%

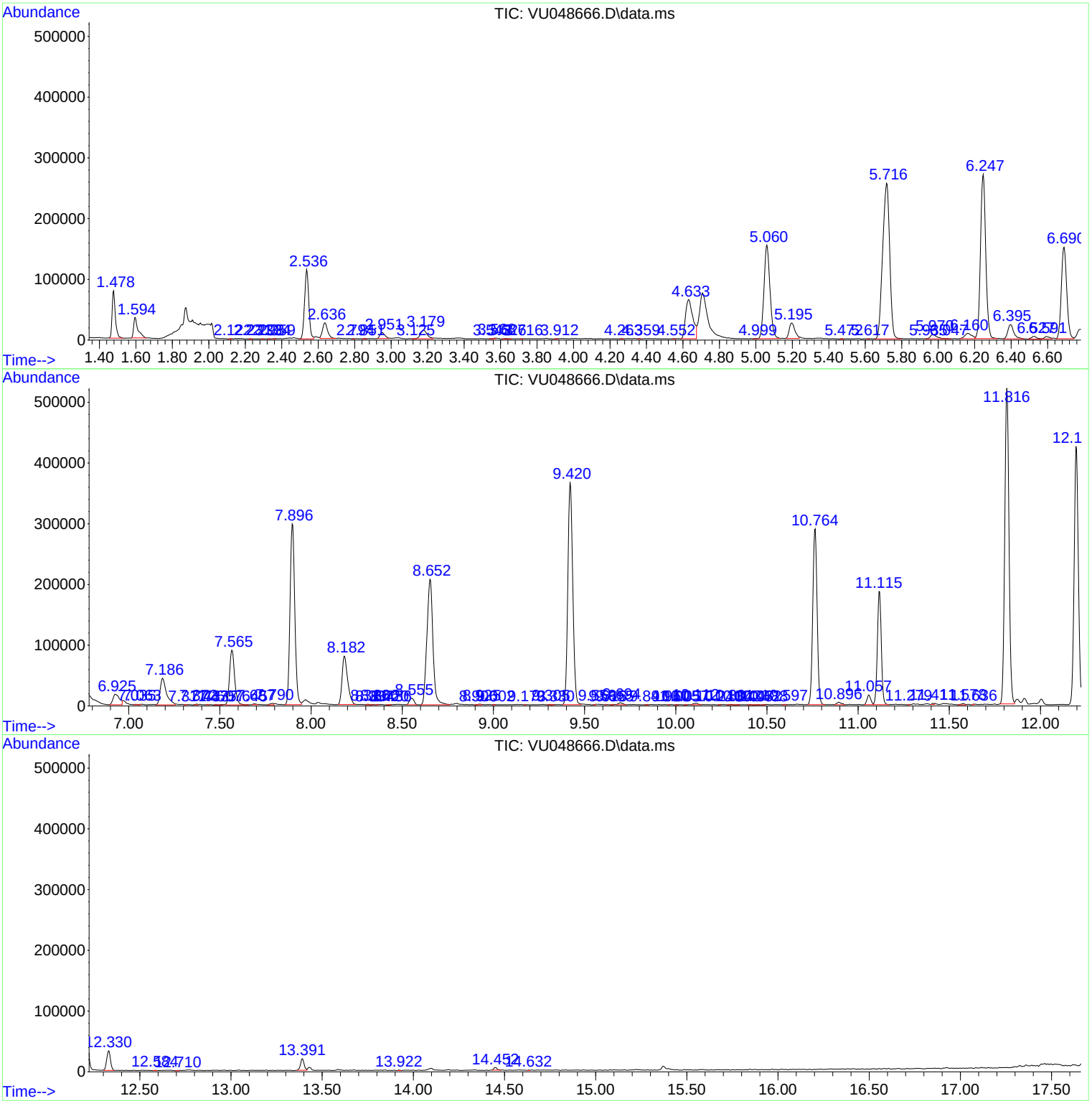
Sum of corrected areas: 7285062

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052522\
Data File : VU048666.D
Acq On : 25 May 2022 13:19
Operator : SY/MD
Sample : N2926-13ME
Misc : 3.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY23ME

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052522\
Data File : VU048666.D
Acq On : 25 May 2022 13:19
Operator : SY/MD
Sample : N2926-13ME
Misc : 3.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY23ME

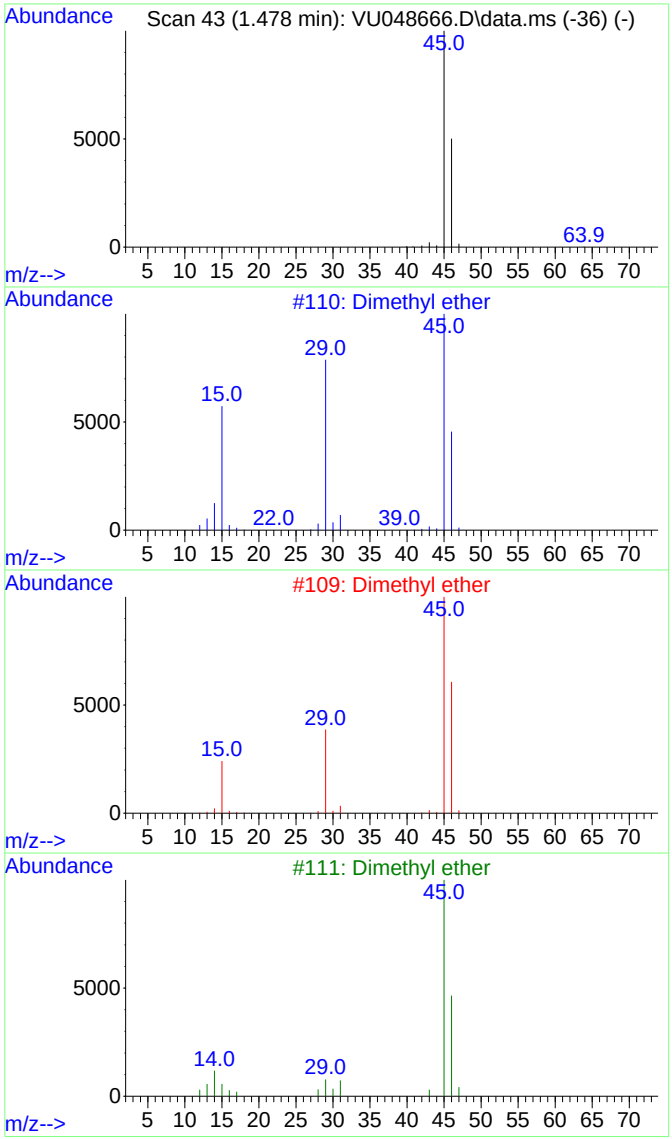
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

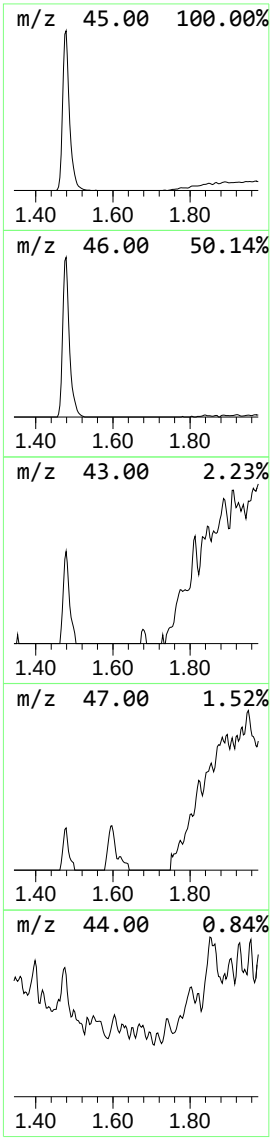
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Dimethyl ether Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.478	8.87 ug/L	95695	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	Dimethyl ether	46	C2H6O	000115-10-6	7
4	Ethanol	46	C2H6O	000064-17-5	7
5	Ethanol	46	C2H6O	000064-17-5	7





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052522\
Data File : VU048666.D
Acq On : 25 May 2022 13:19
Operator : SY/MD
Sample : N2926-13ME
Misc : 3.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY23ME

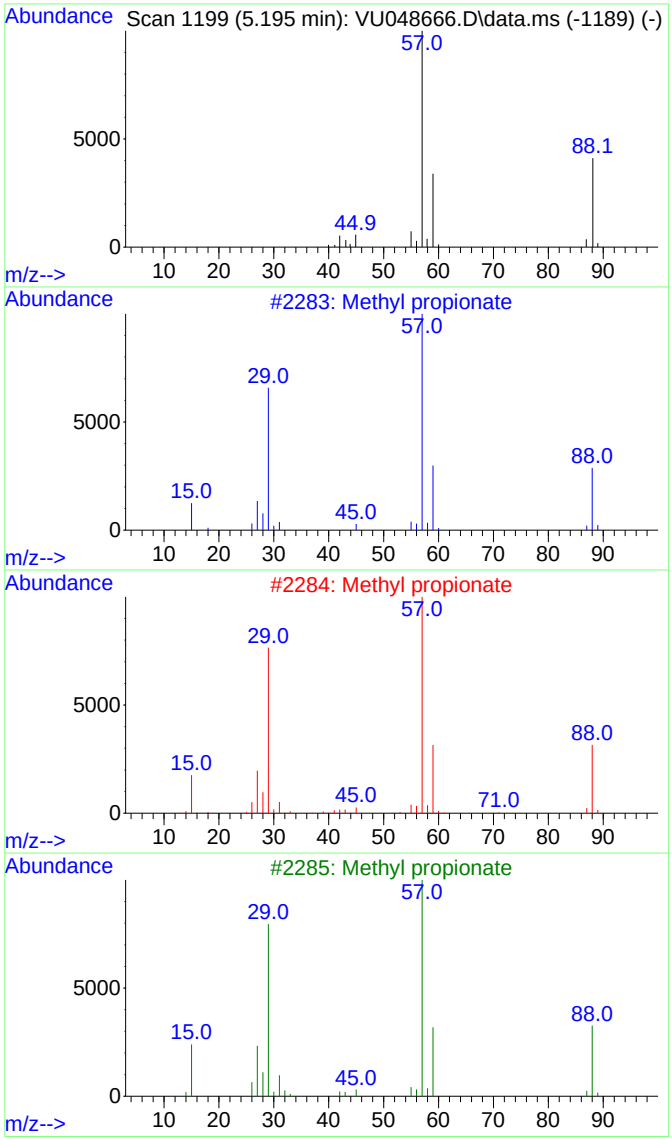
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

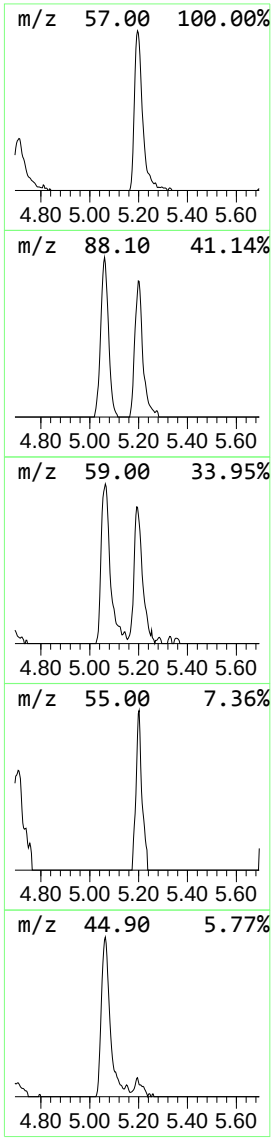
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Methyl propionate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.195	5.09 ug/L	54959	1,4-Difluorobenzene	6.247

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052522\
Data File : VU048666.D
Acq On : 25 May 2022 13:19
Operator : SY/MD
Sample : N2926-13ME
Misc : 3.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY23ME

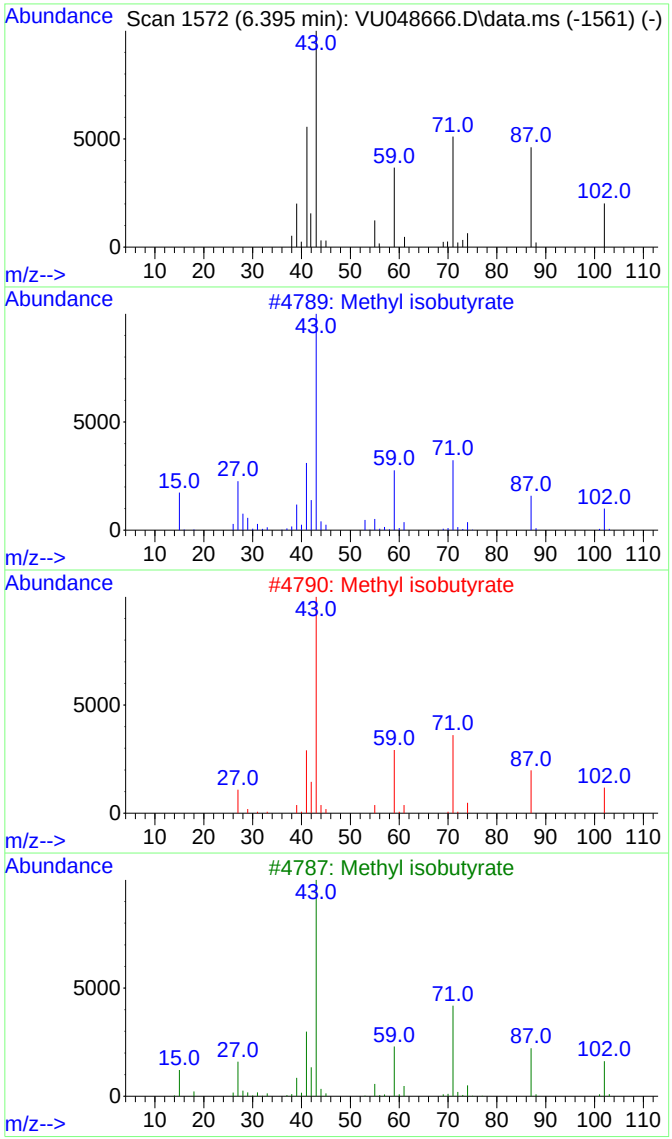
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

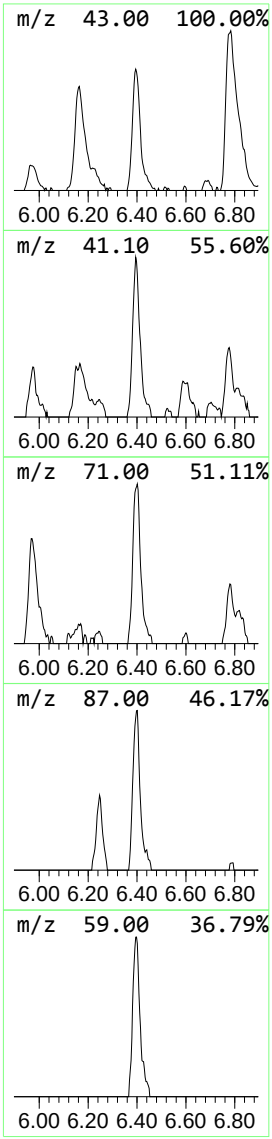
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Methyl isobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.395	4.89 ug/L	52810	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl isobutyrate	102	C5H10O2	000547-63-7	80
2	Methyl isobutyrate	102	C5H10O2	000547-63-7	80
3	Methyl isobutyrate	102	C5H10O2	000547-63-7	80
4	Butyric acid hydrazide	102	C4H10N2O	003538-65-6	38
5	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	28





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052522\
Data File : VU048666.D
Acq On : 25 May 2022 13:19
Operator : SY/MD
Sample : N2926-13ME
Misc : 3.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY23ME

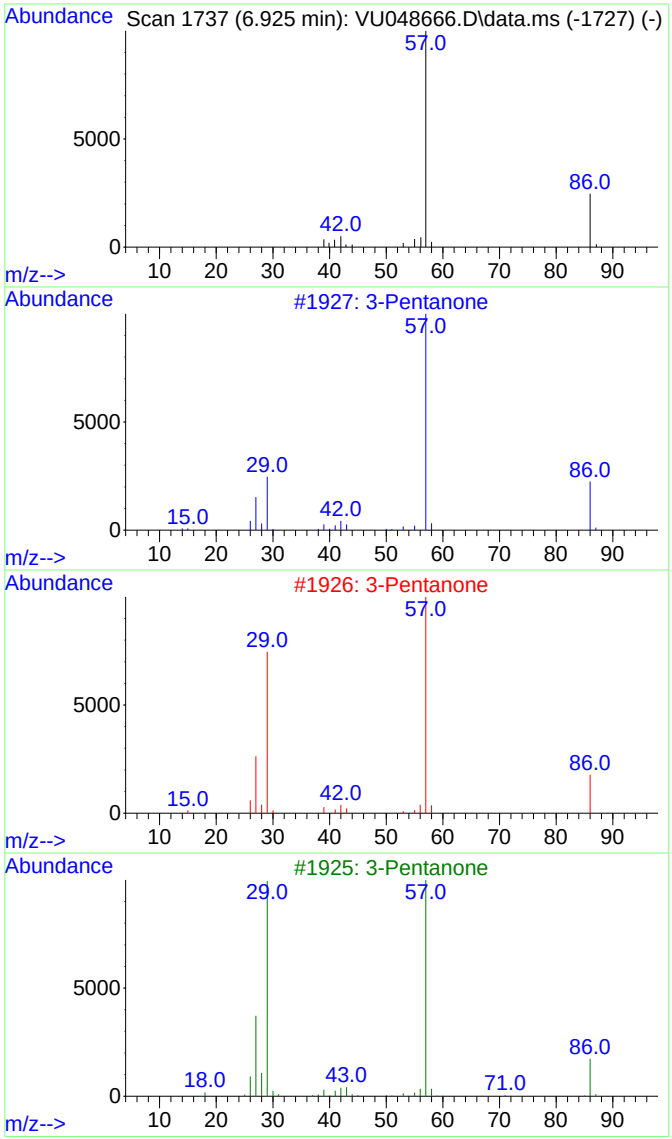
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

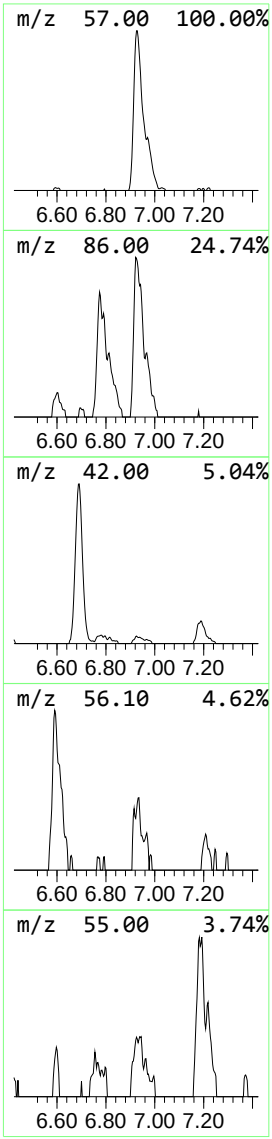
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 3-Pentanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.925	3.96 ug/L	42733	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	72
2	3-Pentanone	86	C5H10O	000096-22-0	56
3	3-Pentanone	86	C5H10O	000096-22-0	56
4	3-Pentanone	86	C5H10O	000096-22-0	50
5	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052522\
Data File : VU048666.D
Acq On : 25 May 2022 13:19
Operator : SY/MD
Sample : N2926-13ME
Misc : 3.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY23ME

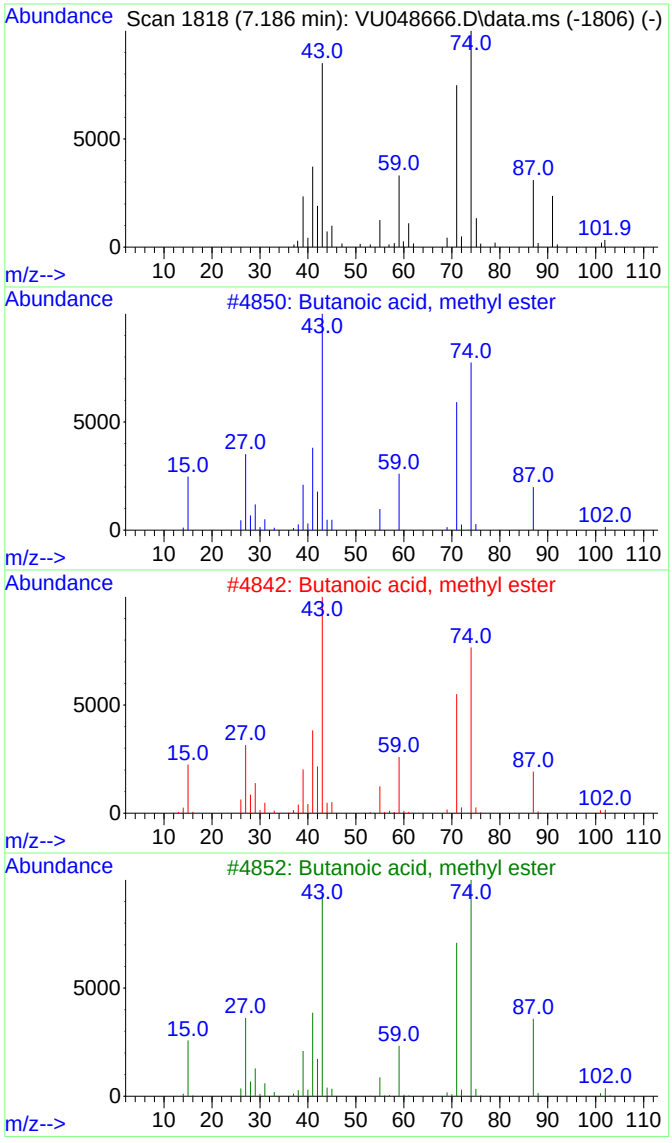
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

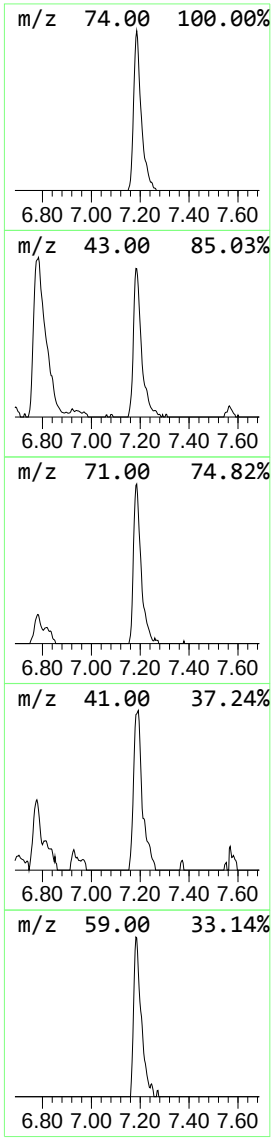
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Butanoic acid, methyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.186	9.57 ug/L	103243	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	90
2	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	90
3	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	87
4	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	80
5	Methyl isobutyrate	102	C5H10O2	000547-63-7	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052522\
Data File : VU048666.D
Acq On : 25 May 2022 13:19
Operator : SY/MD
Sample : N2926-13ME
Misc : 3.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY23ME

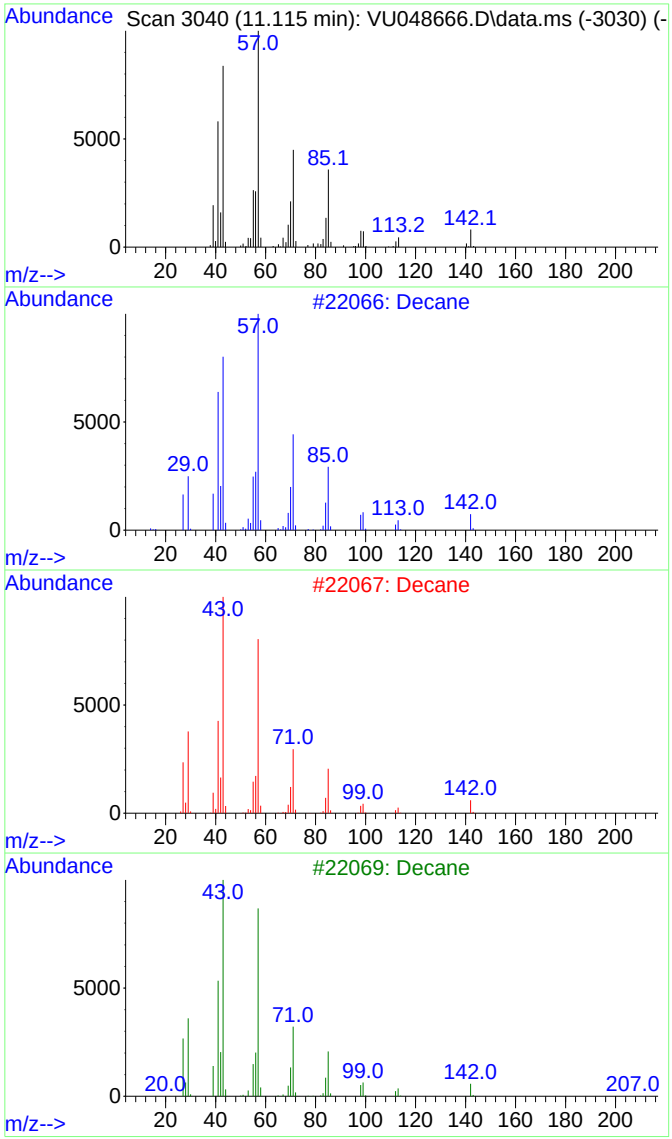
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

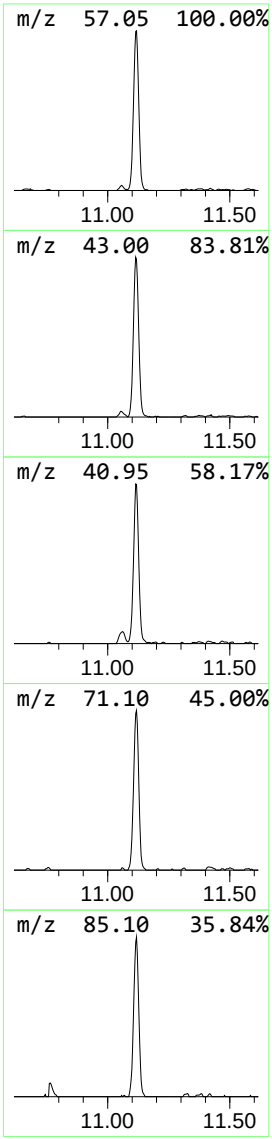
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.115	16.67 ug/L	277567	1,4-Dichlorobenzene-d4	11.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane	142	C10H22	000124-18-5	95
2	Decane	142	C10H22	000124-18-5	95
3	Decane	142	C10H22	000124-18-5	91
4	Decane	142	C10H22	000124-18-5	83
5	Octane	114	C8H18	000111-65-9	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052522\
Data File : VU048666.D
Acq On : 25 May 2022 13:19
Operator : SY/MD
Sample : N2926-13ME
Misc : 3.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY23ME

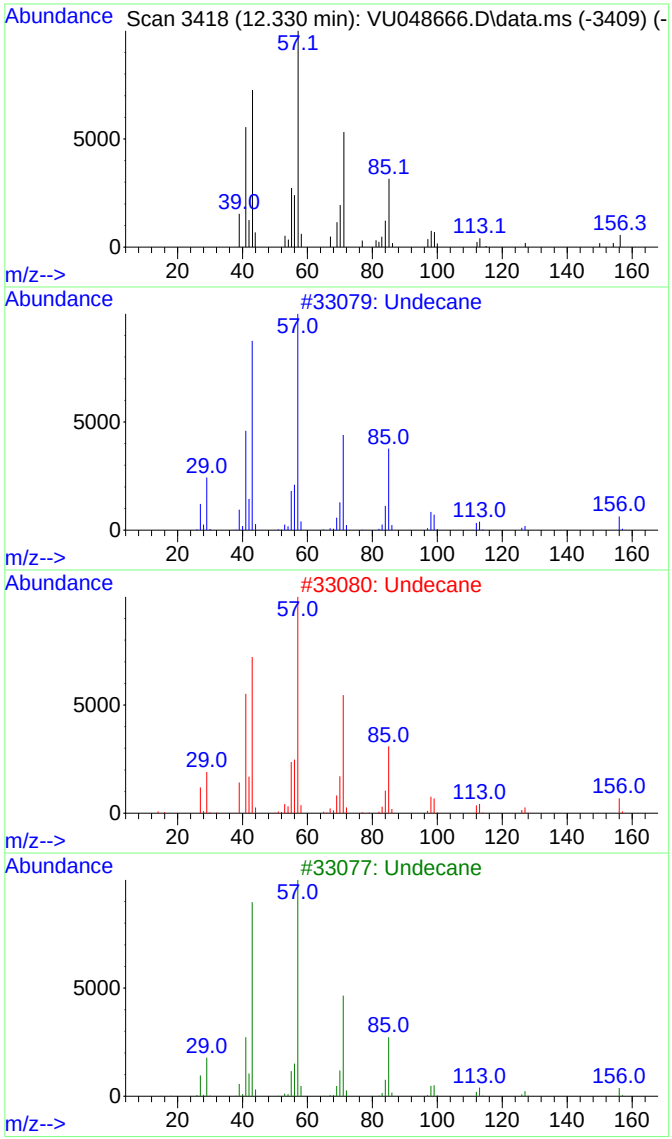
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

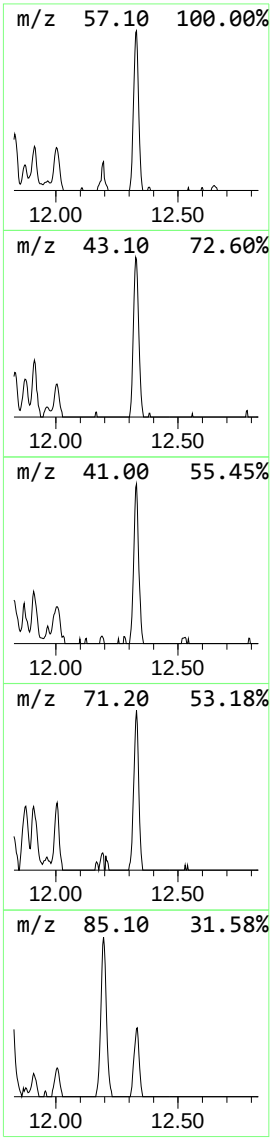
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.330	2.74 ug/L	45601	1,4-Dichlorobenzene-d4	11.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	94
2	Undecane	156	C11H24	001120-21-4	91
3	Undecane	156	C11H24	001120-21-4	87
4	Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	83
5	Decane	142	C10H22	000124-18-5	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052522\
Data File : VU048666.D
Acq On : 25 May 2022 13:19
Operator : SY/MD
Sample : N2926-13ME
Misc : 3.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY23ME

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Dimethyl ether	1.478	8.9	ug/L	95695	1	6.247	539531	50.0
Methyl propionate	5.195	5.1	ug/L	54959	1	6.247	539531	50.0
Methyl isobutyrate	6.395	4.9	ug/L	52810	1	6.247	539531	50.0
3-Pentanone	6.925	4.0	ug/L	42733	1	6.247	539531	50.0
Butanoic acid, ...	7.186	9.6	ug/L	103243	1	6.247	539531	50.0
(DEL) Alkane: S...	11.115	16.7	ug/L	277567	3	11.816	832651	50.0
(DEL) Alkane: S...	12.330	2.7	ug/L	45601	3	11.816	832651	50.0