LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052322\
Data File : VU048658.D
Acq On : 23 May 2022 18:09
Operator : SY/MD
Sample : N2926-07ME
Misc : 4.52g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY16ME

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: VU048658.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	61	rBV	37569	47915	5.68%	0.626%
2	1.594	73	79	86	rBV	36722	47134	5.59%	0.616%
3	2.240	278	280	283	rBV	367	225	0.03%	0.003%
4	2.317	302	304	310	rBV	292	286	0.03%	0.004%
5	2.353	312	315	316	rBV	557	287	0.03%	0.004%
6	2.530	358	370	383	rBV	129912	211711	25.12%	2.766%
7	2.639	396	404	423	rVB4	25842	51335	6.09%	0.671%
8	2.745	435	437	440	rBV	645	462	0.05%	0.006%
9	2.822	458	461	466	rBV	187	231	0.03%	0.003%
10	2.957	490	503	516	rBV3	4858	9910	1.18%	0.129%
11	3.025	521	524	528	rBV4	1085	902	0.11%	0.012%
12	3.176	559	571	585	rBV	7197	17135	2.03%	0.224%
13	3.276	600	602	607	rVB2	384	300	0.04%	0.004%
14	3.301	607	610	614	rVB	382	284	0.03%	0.004%
15	3.366	625	630	635	rBV2	604	704	0.08%	0.009%
16	3.449	654	656	662	rBB	261	255	0.03%	0.003%
17	3.562	685	691	692	rBV3	667	587	0.07%	0.008%
18	3.951	809	812	815	rBV3	418	346	0.04%	0.005%
19	4.028	833	836	840	rBV2	236	235	0.03%	0.003%
20	4.057	840	845	848	rBV2	650	680	0.08%	0.009%
21	4.105	857	860	862	rVB2	357	225	0.03%	0.003%
22	4.433	958	962	965	rBB	329	235	0.03%	0.003%
23	4.449	965	967	972	rBV	277	241	0.03%	0.003%
24	4.636	1010	1025	1037	rBV	68507	186720	22.15%	2.439%
25	4.970	1125	1129	1131	rBV2	313	227	0.03%	0.003%
26	5.060	1141	1157	1184	rBV	165191	383979	45.55%	5.016%
27	5.198	1188	1200	1220	rBV2	26581	60418	7.17%	0.789%
28	5.321	1234	1238	1240	rBV2	954	733	0.09%	0.010%
29	5.716	1339	1361	1384	rBV2	286000	761596	90.35%	9.949%
30	5.973	1429	1441	1455	rBV4	8473	19841	2.35%	0.259%
31	6.054	1464	1466	1472	rVB	376	210	0.02%	0.003%
32	6.115	1481	1485	1486	rBV	391	299	0.04%	0.004%
33	6.160	1488	1499	1512	rVV4	10438	27036	3.21%	0.353%
34	6.247	1514	1526	1547	rVB	277754	557692	66.16%	7.286%
35	6.398	1560	1573	1588	rBV3	27293	56414	6.69%	0.737%
36	6.523	1602	1612	1622	rBV4	4304	8000	0.95%	0.105%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052322\
Data File : VU048658.D
Acq On : 23 May 2022 18:09
Operator : SY/MD
Sample : N2926-07ME
Misc : 4.52g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY16ME

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	6.597	1625	1635	1649	rBV7	4535	10518	1.25%	0.137%
38	6.690	1649	1664	1682	rVV	169189	343652	40.77%	4.489%
39	6.780	1682	1692	1719	rVB2	17295	53580	6.36%	0.700%
40	6.928	1728	1738	1761	rBV	19674	51224	6.08%	0.669%
41	7.041	1770	1773	1775	rBV	389	242	0.03%	0.003%
42	7.185	1807	1818	1842	rBV5	49427	111856	13.27%	1.461%
43	7.327	1859	1862	1865	rBV2	392	316	0.04%	0.004%
44	7.439	1893	1897	1899	rBV	275	293	0.03%	0.004%
45	7.565	1924	1936	1958	rVB	99234	188758	22.39%	2.466%
46	7.693	1969	1976	1980	rVV3	1121	1469	0.17%	0.019%
47	7.716	1980	1983	1987	rVV2	546	449	0.05%	0.006%
48	7.790	1997	2006	2007	rBV2	1669	1886	0.22%	0.025%
49	7.899	2025	2040	2055	rBV	331081	598608	71.02%	7.820%
50	8.108	2103	2105	2107	rBV	664	434	0.05%	0.006%
51	8.182	2116	2128	2156	rVB2	90345	189702	22.51%	2.478%
52	8.288	2157	2161	2165	rBV2	378	466	0.06%	0.006%
53	8.353	2176	2181	2184	rBV	521	436	0.05%	0.006%
54	8.459	2210	2214	2216	rBV2	418	312	0.04%	0.004%
55	8.488	2222	2223	2227	rVB	532	289	0.03%	0.004%
56	8.520	2228	2233	2235	rBV	348	225	0.03%	0.003%
57	8.549	2239	2242	2249	rVB3	675	649	0.08%	0.008%
58	8.652	2258	2274	2308	rBV	231289	516546	61.28%	6.748%
59	8.902	2349	2352	2355	rBV	356	275	0.03%	0.004%
60	8.925	2355	2359	2361	rBV2	467	450	0.05%	0.006%
61	9.156	2428	2431	2435	rVV2	333	273	0.03%	0.004%
62	9.221	2445	2451	2454	rBB	259	304	0.04%	0.004%
63	9.420	2500	2513	2529	rBV	383356	706445	83.81%	9.229%
64	9.555	2550	2555	2558	rBV2	444	469	0.06%	0.006%
65	9.616	2570	2574	2577	rBV	222	234	0.03%	0.003%
66	9.693	2588	2598	2600	rBV5	2752	3183	0.38%	0.042%
67	9.748	2613	2615	2620	rVB	357	279	0.03%	0.004%
68	10.079	2712	2718	2720	rBV	277	284	0.03%	0.004%
69	10.105	2720	2726	2735	rVV5	2175	3258	0.39%	0.043%
70	10.217	2759	2761	2765	rVB	361	221	0.03%	0.003%
71	10.664	2898	2900	2903	rVV	500	278	0.03%	0.004%
72	10.764	2918	2931	2948	rBV	314313	514346	61.02%	6.719%
73	11.005	3002	3006	3009	rVB3	447	327	0.04%	0.004%
74	11.060	3014	3023	3030	rVV4	11398	16353	1.94%	0.214%
75	11.118	3030	3041	3055	rVV	138506	207156	24.58%	2.706%
76	11.172	3055	3058	3062	rVB3	411	320	0.04%	0.004%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052322\
Data File : VU048658.D
Acq On : 23 May 2022 18:09
Operator : SY/MD
Sample : N2926-07ME
Misc : 4.52g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY16ME

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	11.221	3070	3073	3078	rVB3	441	345	0.04%	0.005%
78	11.317	3099	3103	3112	rVB4	889	924	0.11%	0.012%
79	11.375	3114	3121	3128	rVB4	1419	1621	0.19%	0.021%
80	11.417	3128	3134	3136	rBV2	1350	1199	0.14%	0.016%
81	11.475	3142	3152	3157	rBV6	1543	2557	0.30%	0.033%
82	11.574	3177	3183	3189	rBV3	957	1387	0.16%	0.018%
83	11.635	3198	3202	3204	rBV2	439	312	0.04%	0.004%
84	11.697	3217	3221	3227	rVB4	845	762	0.09%	0.010%
85	11.754	3231	3239	3243	rBV4	1313	1801	0.21%	0.024%
86	11.815	3243	3258	3271	rBV	529701	842908	100.00%	11.012%
87	12.005	3312	3317	3327	rVB5	6785	9294	1.10%	0.121%
88	12.095	3341	3345	3350	rBV2	275	239	0.03%	0.003%
89	12.198	3364	3377	3391	rBV	453885	731101	86.74%	9.551%
90	12.330	3408	3418	3427	rBV2	25374	35818	4.25%	0.468%
91	12.471	3458	3462	3468	rVB2	289	318	0.04%	0.004%
92	12.648	3515	3517	3523	rVB2	331	262	0.03%	0.003%
93	12.764	3551	3553	3555	rBV3	529	312	0.04%	0.004%
94	13.227	3690	3697	3702	rBV4	1283	1541	0.18%	0.020%
95	13.391	3739	3748	3757	rBV5	14743	20497	2.43%	0.268%
96	13.684	3836	3839	3841	rBV2	339	212	0.03%	0.003%
97	13.729	3850	3853	3856	rBV	272	211	0.03%	0.003%
98	14.092	3958	3966	3977	rVB2	9148	14701	1.74%	0.192%
99	14.330	4037	4040	4041	rBV	1232	708	0.08%	0.009%
100	15.233	4313	4321	4330	rBV6	2266	4570	0.54%	0.060%

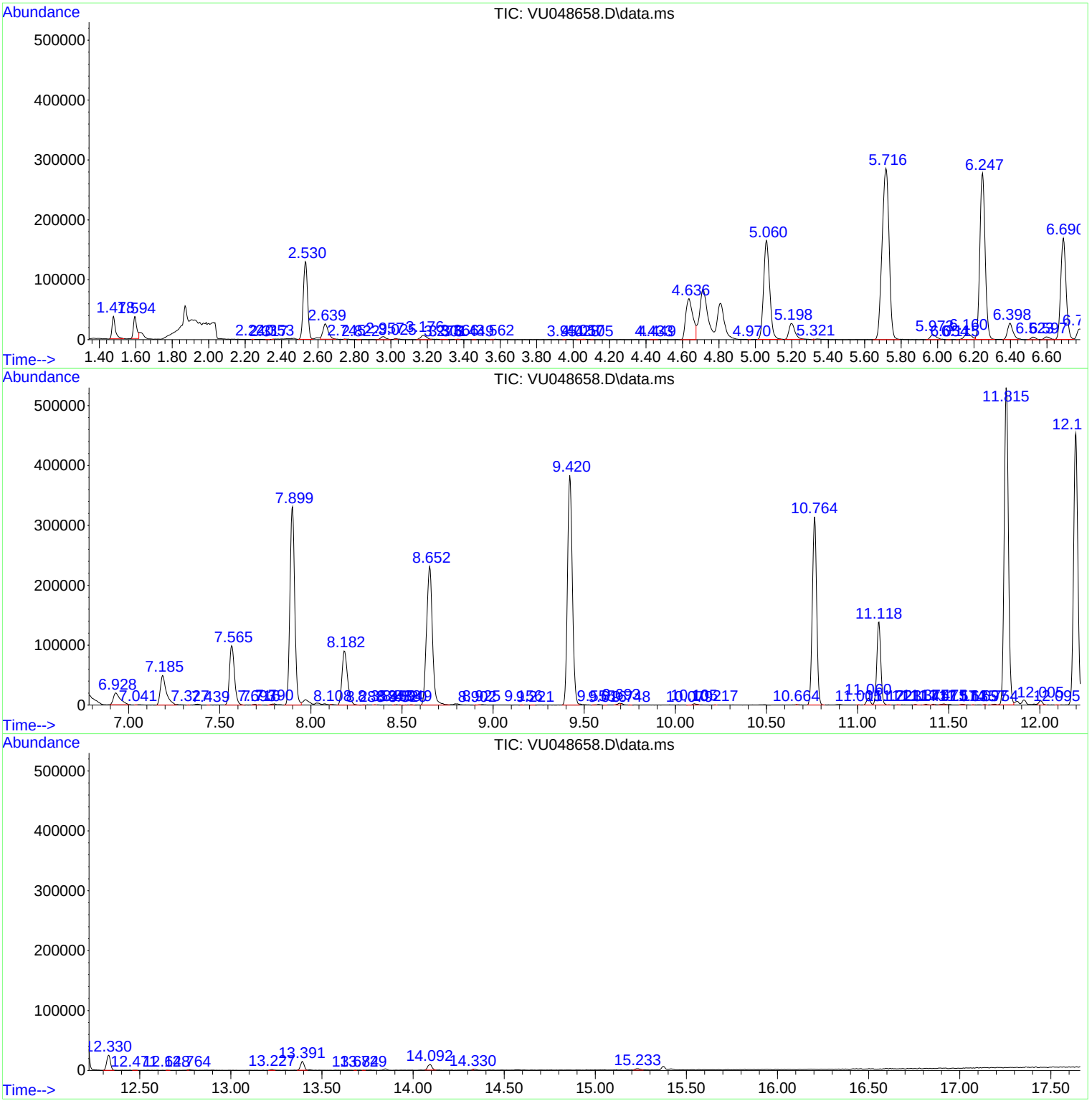
Sum of corrected areas: 7654755

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052322\
Data File : VU048658.D
Acq On : 23 May 2022 18:09
Operator : SY/MD
Sample : N2926-07ME
Misc : 4.52g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY16ME

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\VU052322\
Data File : VU048658.D
Acq On : 23 May 2022 18:09
Operator : SY/MD
Sample : N2926-07ME
Misc : 4.52g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY16ME

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

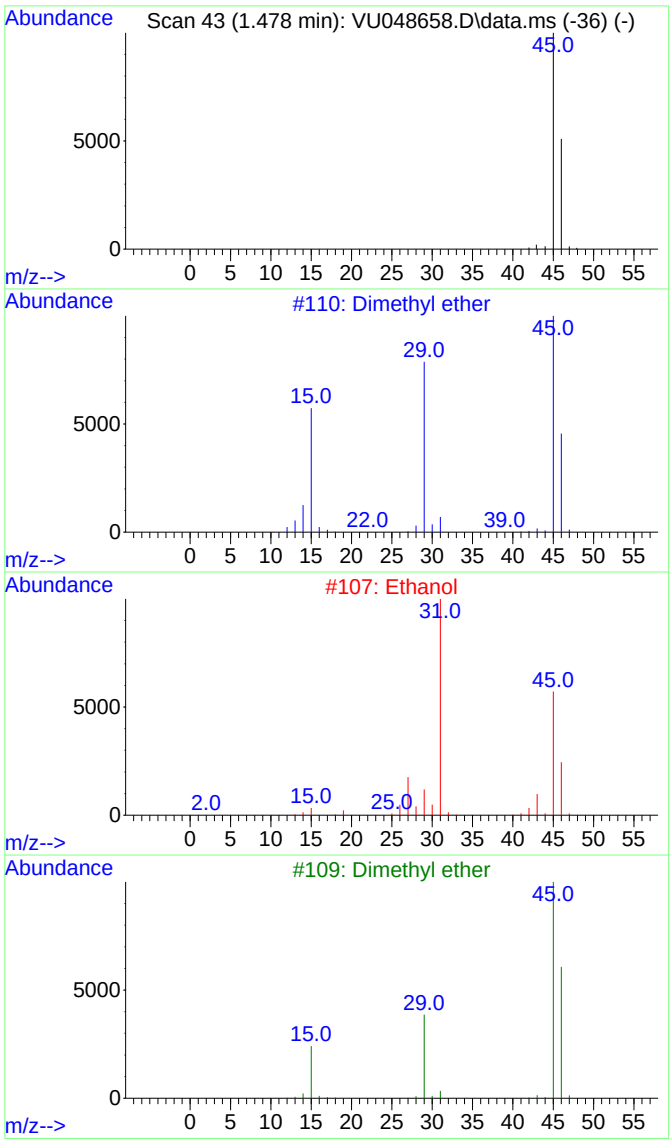
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

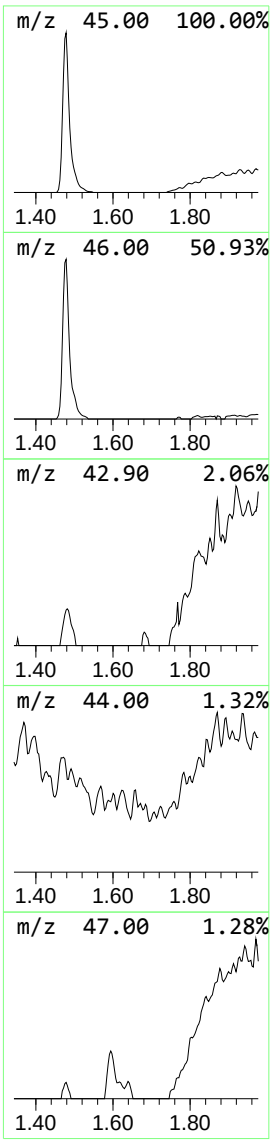
****

Peak Number 1 Dimethyl ether Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.478	4.30 ug/L	47915	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl ether	46	C2H6O	000115-10-6	90
2	Ethanol	46	C2H6O	000064-17-5	9
3	Dimethyl ether	46	C2H6O	000115-10-6	9
4	Ethanol	46	C2H6O	000064-17-5	7
5	Dimethyl ether	46	C2H6O	000115-10-6	5





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052322\
Data File : VU048658.D
Acq On : 23 May 2022 18:09
Operator : SY/MD
Sample : N2926-07ME
Misc : 4.52g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY16ME

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

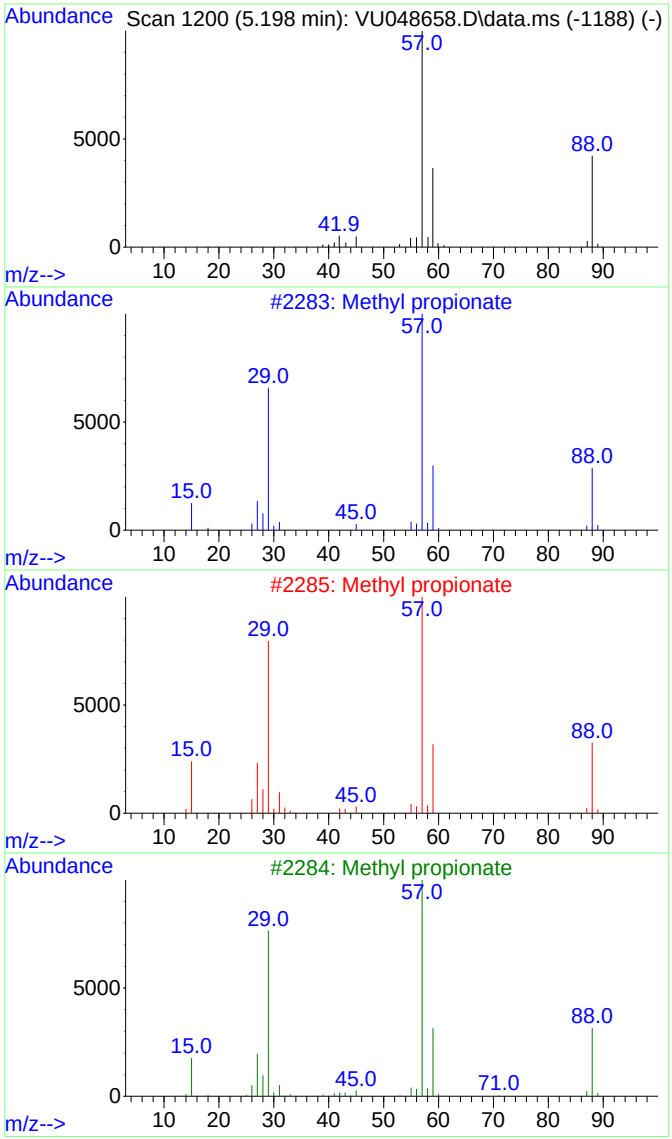
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

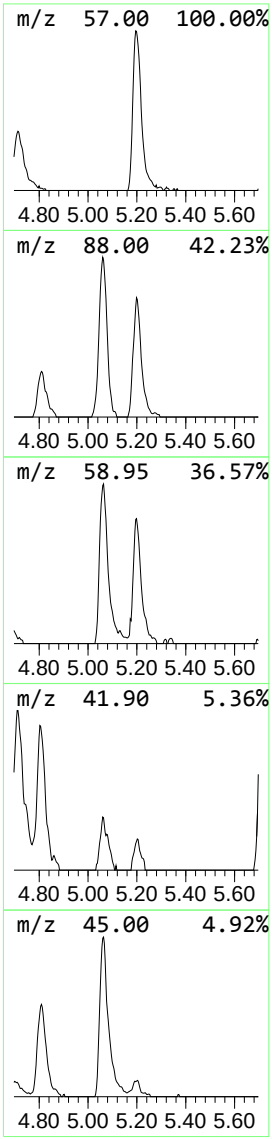
****

Peak Number 2 Methyl propionate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.198	5.42 ug/L	60418	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	86
4	Methyl propionate	88	C4H8O2	000554-12-1	83
5	Methyl propionate	88	C4H8O2	000554-12-1	80





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052322\
Data File : VU048658.D
Acq On : 23 May 2022 18:09
Operator : SY/MD
Sample : N2926-07ME
Misc : 4.52g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY16ME

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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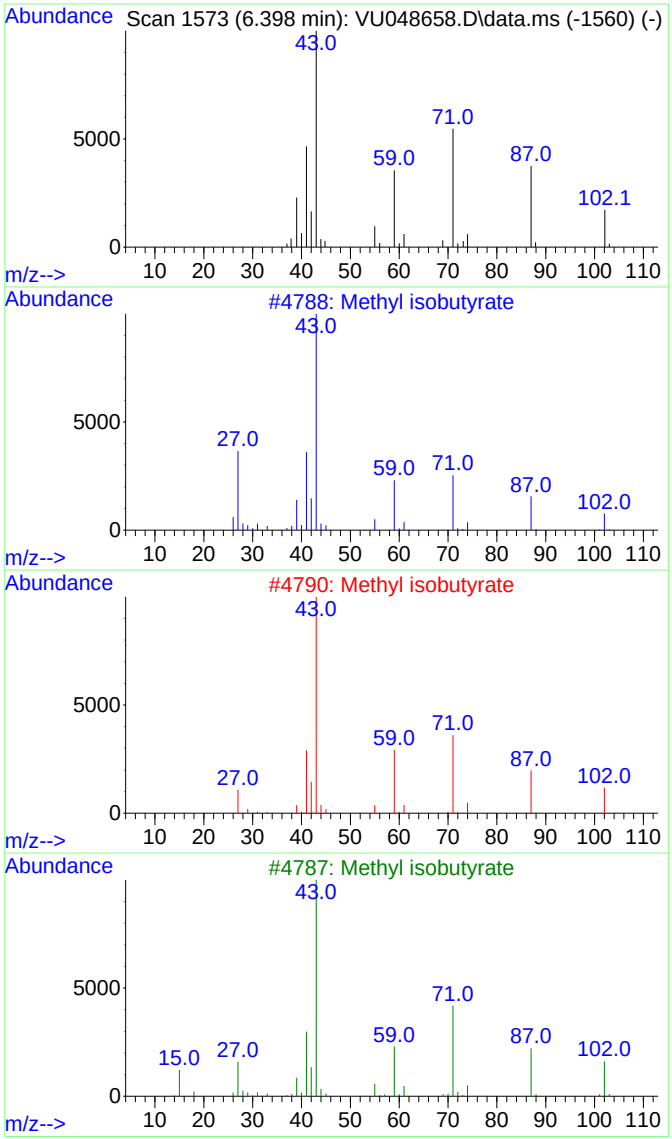
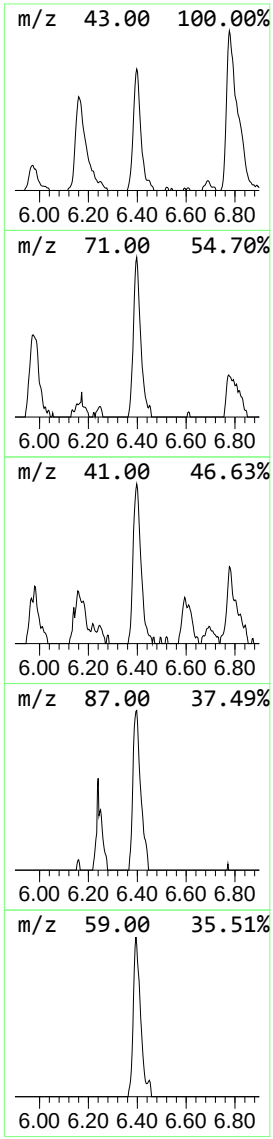
Peak Number 3 Methyl isobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.398	5.06 ug/L	56414	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	90
3	Methyl isobutyrate	102	C5H10O2	000547-63-7	72
4	Methyl isobutyrate	102	C5H10O2	000547-63-7	64
5	Butyric acid hydrazide	102	C4H10N2O	003538-65-6	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052322\
Data File : VU048658.D
Acq On : 23 May 2022 18:09
Operator : SY/MD
Sample : N2926-07ME
Misc : 4.52g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY16ME

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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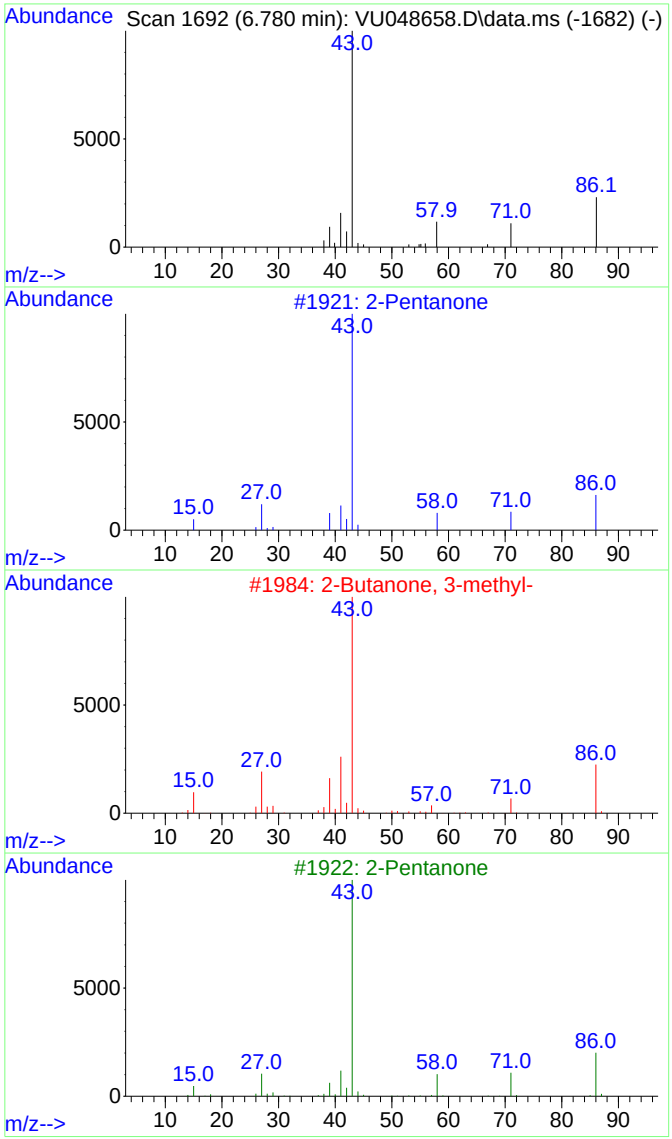
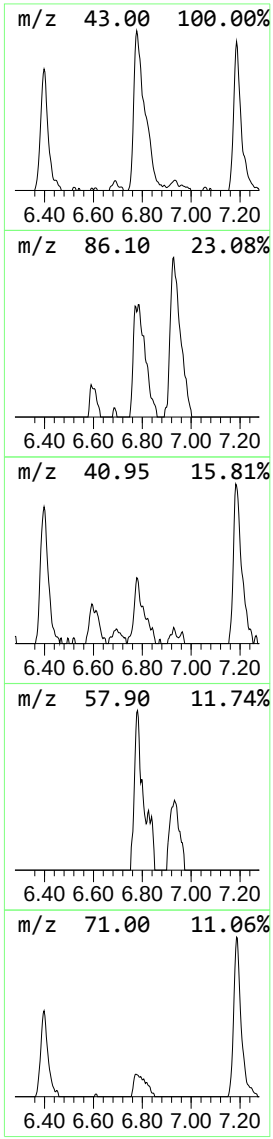
Peak Number 4 2-Pentanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.780	4.80 ug/L	53580	1,4-Difluorobenzene	6.247

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052322\
Data File : VU048658.D
Acq On : 23 May 2022 18:09
Operator : SY/MD
Sample : N2926-07ME
Misc : 4.52g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY16ME

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

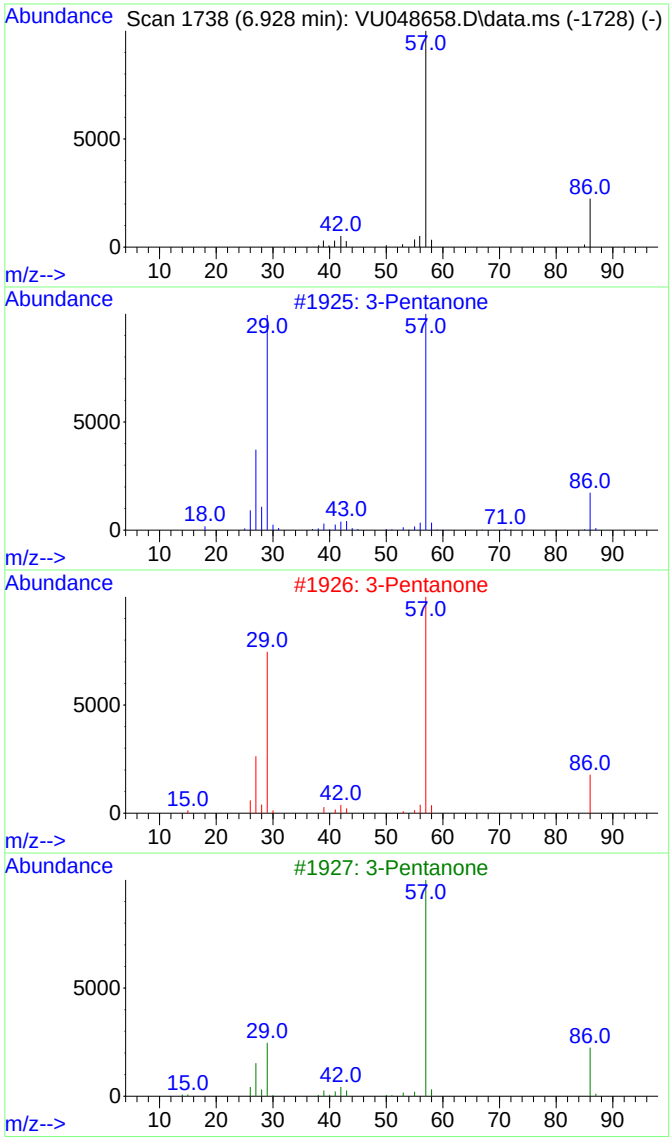
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

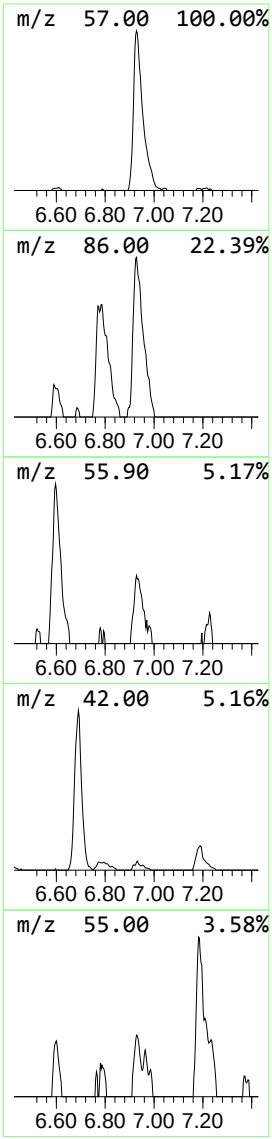
****

Peak Number 5 3-Pentanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.928	4.59 ug/L	51224	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	78
2	3-Pentanone	86	C5H10O	000096-22-0	72
3	3-Pentanone	86	C5H10O	000096-22-0	64
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\VU052322\
Data File : VU048658.D
Acq On : 23 May 2022 18:09
Operator : SY/MD
Sample : N2926-07ME
Misc : 4.52g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY16ME

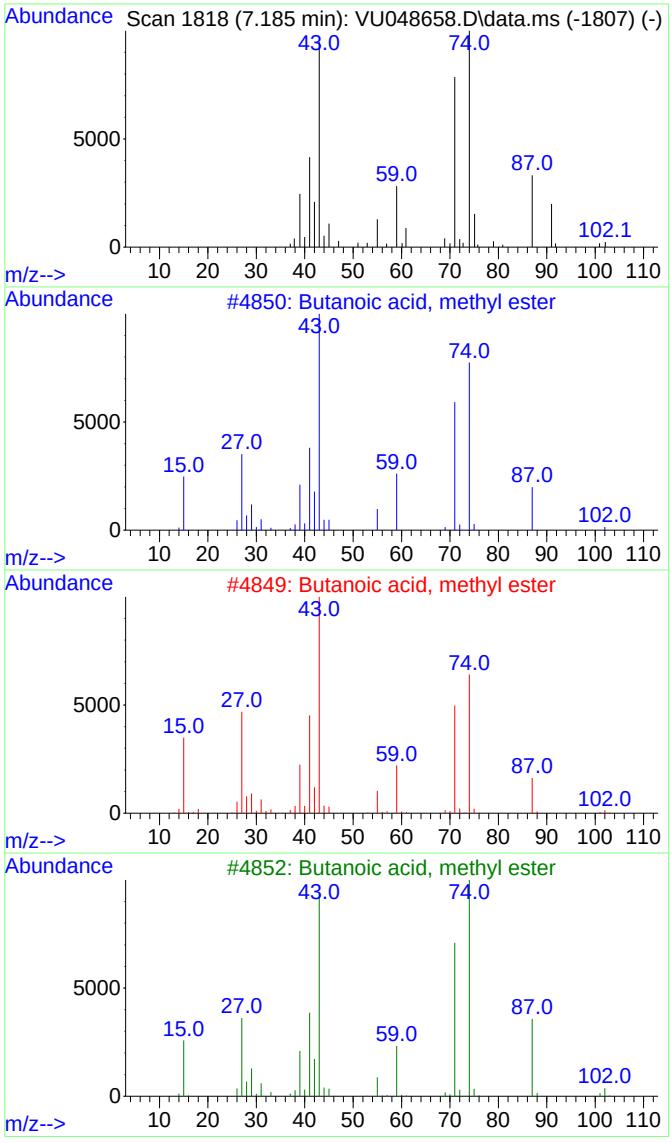
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

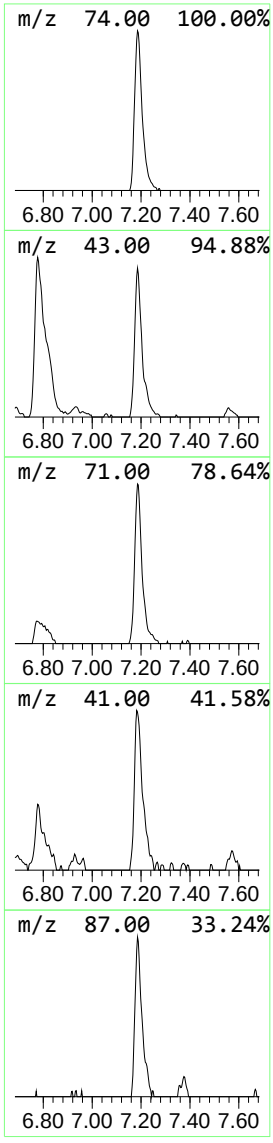
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.185	10.03 ug/L	111856	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	83
2	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	80
3	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	78
4	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	58
5	Methyl isobutyrate	102	C5H10O2	000547-63-7	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052322\
Data File : VU048658.D
Acq On : 23 May 2022 18:09
Operator : SY/MD
Sample : N2926-07ME
Misc : 4.52g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY16ME

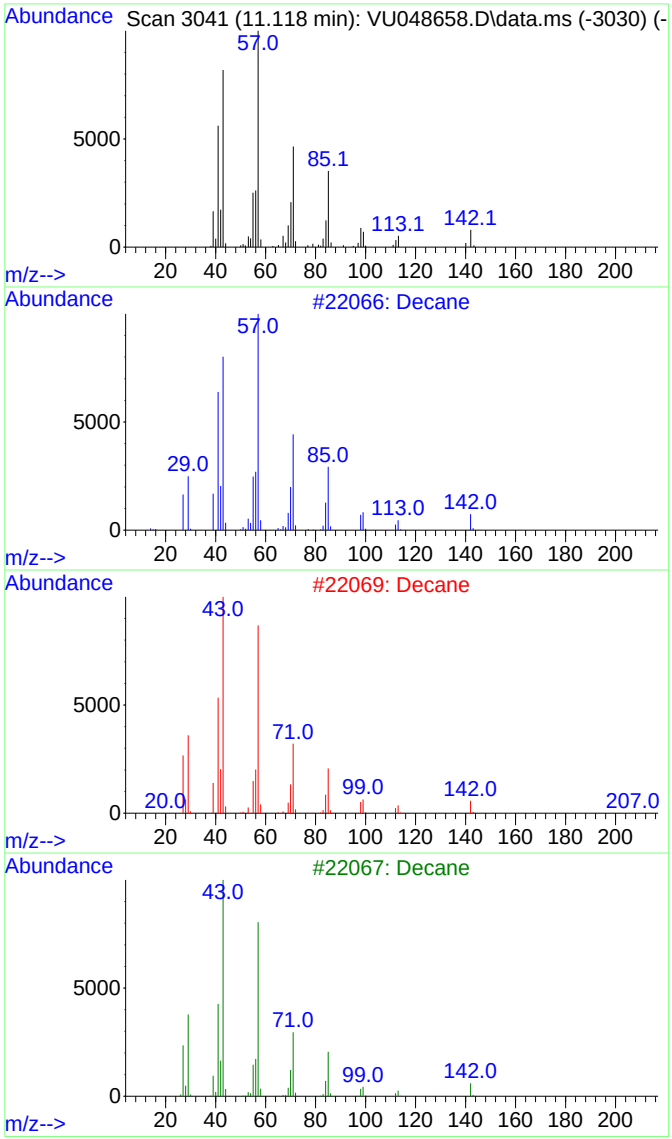
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

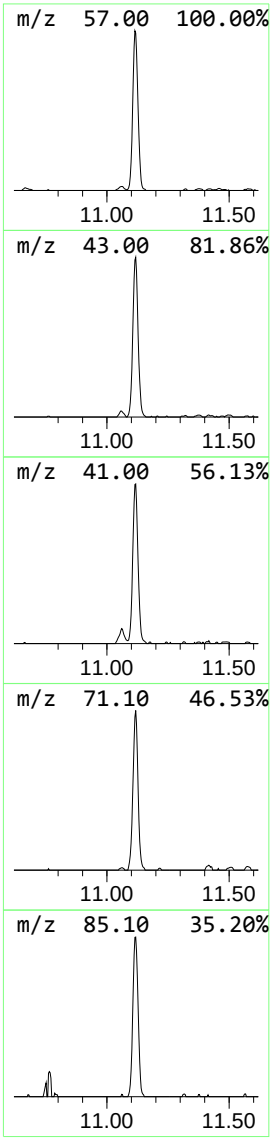
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.118	12.29 ug/L	207156	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	94
3	Decane	142	C10H22	000124-18-5	91
4	Decane	142	C10H22	000124-18-5	87
5	Octane	114	C8H18	000111-65-9	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052322\
Data File : VU048658.D
Acq On : 23 May 2022 18:09
Operator : SY/MD
Sample : N2926-07ME
Misc : 4.52g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY16ME

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	4.3	ug/L	47915	1	6.247	557692	50.0
Methyl propionate	5.198	5.4	ug/L	60418	1	6.247	557692	50.0
Methyl isobutyrate	6.398	5.1	ug/L	56414	1	6.247	557692	50.0
2-Pentanone	6.780	4.8	ug/L	53580	1	6.247	557692	50.0
3-Pentanone	6.928	4.6	ug/L	51224	1	6.247	557692	50.0
Butanoic acid, ...	7.185	10.0	ug/L	111856	1	6.247	557692	50.0
(DEL) Alkane: S...	11.118	12.3	ug/L	207156	3	11.816	842908	50.0