LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050222\
Data File : VU048374.D
Acq On : 02 May 2022 17:31
Operator : SY/MD
Sample : N2638-08
Misc : 5.36g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL03

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\SFAMULM042522WMA.M
Title : VOC Analysis

Signal : TIC: VU048374.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.479	34	43	71	rBV	203732	402338	15.95%	1.943%
2	1.597	74	80	86	rBV	77888	118577	4.70%	0.573%
3	2.530	357	370	385	rBV	341263	627949	24.90%	3.032%
4	2.858	469	472	473	rBV2	585	352	0.01%	0.002%
5	2.961	493	504	516	rBV2	9138	22053	0.87%	0.106%
6	3.179	559	572	587	rBV	18526	43852	1.74%	0.212%
7	3.366	623	630	633	rBV3	819	978	0.04%	0.005%
8	3.453	651	657	658	rBV2	655	627	0.02%	0.003%
9	3.485	665	667	671	rVB	521	332	0.01%	0.002%
10	3.504	671	673	679	rVB3	521	428	0.02%	0.002%
11	3.549	679	687	688	rBV3	1818	1531	0.06%	0.007%
12	3.613	705	707	711	rVB3	794	446	0.02%	0.002%
13	3.642	713	716	718	rBV2	618	379	0.02%	0.002%
14	3.755	748	751	755	rVB	501	328	0.01%	0.002%
15	3.832	770	775	777	rBV	932	857	0.03%	0.004%
16	3.858	777	783	784	rBV3	652	640	0.03%	0.003%
17	3.893	792	794	798	rVB	575	353	0.01%	0.002%
18	4.015	828	832	834	rBV2	520	446	0.02%	0.002%
19	4.060	842	846	847	rBV2	612	475	0.02%	0.002%
20	4.125	863	866	876	rVB2	998	1318	0.05%	0.006%
21	4.173	876	881	884	rBV	776	600	0.02%	0.003%
22	4.205	888	891	897	rBV	287	403	0.02%	0.002%
23	4.234	897	900	905	rVB2	766	570	0.02%	0.003%
24	4.366	938	941	945	rVB	654	456	0.02%	0.002%
25	4.404	950	953	956	rBV2	620	541	0.02%	0.003%
26	4.427	956	960	963	rBV	605	529	0.02%	0.003%
27	4.456	966	969	971	rBV3	515	330	0.01%	0.002%
28	4.488	975	979	985	rVB3	812	758	0.03%	0.004%
29	4.523	986	990	992	rBV2	586	472	0.02%	0.002%
30	4.642	1008	1027	1039	rBV	180636	571272	22.65%	2.758%
31	5.064	1140	1158	1188	rBV	432293	1125011	44.60%	5.432%
32	5.202	1190	1201	1232	rVB	55477	147411	5.84%	0.712%
33	5.385	1255	1258	1265	rVB	1093	1260	0.05%	0.006%
34	5.420	1265	1269	1272	rBV2	660	522	0.02%	0.003%
35	5.456	1277	1280	1285	rVB2	551	424	0.02%	0.002%
36	5.501	1291	1294	1298	rBV2	517	439	0.02%	0.002%

LSC Area Percent Report

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Operator : SY/MD
Sample : N2638-08
Misc : 5.36g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL03

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\SFAMULM042522WMA.M
Title : VOC Analysis

37	5.549	1305	1309	1314	rBV	361	328	0.01%	0.002%
38	5.584	1317	1320	1324	rVV3	681	590	0.02%	0.003%
39	5.620	1328	1331	1334	rBV2	438	376	0.01%	0.002%
40	5.716	1340	1361	1390	rBV2	998677	2522339	100.00%	12.178%
41	5.977	1430	1442	1458	rBV4	17835	47772	1.89%	0.231%
42	6.163	1481	1500	1502	rBV	20194	31587	1.25%	0.153%
43	6.247	1513	1526	1561	rVB	479109	1029475	40.81%	4.971%
44	6.398	1561	1573	1599	rVB2	50480	123262	4.89%	0.595%
45	6.488	1599	1601	1604	rBV3	555	355	0.01%	0.002%
46	6.530	1604	1614	1625	rVB5	4703	8829	0.35%	0.043%
47	6.601	1626	1636	1649	rBV7	9076	22565	0.89%	0.109%
48	6.691	1650	1664	1683	rVV	533852	1169070	46.35%	5.645%
49	6.784	1685	1693	1726	rVV	33306	131724	5.22%	0.636%
50	6.935	1728	1740	1774	rVB2	36572	130112	5.16%	0.628%
51	7.189	1804	1819	1852	rBV3	86849	245162	9.72%	1.184%
52	7.568	1923	1937	1963	rBV	275192	594180	23.56%	2.869%
53	7.899	2025	2040	2056	rBV	1075354	2063503	81.81%	9.963%
54	8.186	2116	2129	2161	rVB2	213258	509051	20.18%	2.458%
55	8.346	2176	2179	2180	rBV3	1003	625	0.02%	0.003%
56	8.552	2231	2243	2258	rBV2	112035	195177	7.74%	0.942%
57	8.662	2259	2277	2310	rBV	687190	1658657	65.76%	8.008%
58	9.096	2407	2412	2416	rBV2	732	869	0.03%	0.004%
59	9.166	2431	2434	2435	rBV2	557	340	0.01%	0.002%
60	9.289	2469	2472	2475	rBV3	601	421	0.02%	0.002%
61	9.324	2480	2483	2486	rBV	830	569	0.02%	0.003%
62	9.424	2499	2514	2539	rBV	615294	1284782	50.94%	6.203%
63	9.697	2593	2599	2610	rVB3	6634	11506	0.46%	0.056%
64	9.742	2610	2613	2617	rVB3	699	554	0.02%	0.003%
65	9.957	2678	2680	2683	rBV	729	463	0.02%	0.002%
66	10.041	2703	2706	2712	rBV2	566	467	0.02%	0.002%
67	10.105	2720	2726	2737	rVB4	3715	6242	0.25%	0.030%
68	10.179	2745	2749	2751	rBV2	524	414	0.02%	0.002%
69	10.195	2751	2754	2758	rVV	546	419	0.02%	0.002%
70	10.382	2809	2812	2817	rVB2	599	536	0.02%	0.003%
71	10.440	2827	2830	2835	rBV	710	466	0.02%	0.002%
72	10.485	2840	2844	2846	rBV2	558	507	0.02%	0.002%
73	10.530	2853	2858	2860	rBV2	985	785	0.03%	0.004%
74	10.668	2895	2901	2912	rVB5	3287	5672	0.22%	0.027%
75	10.768	2917	2932	2949	rVV	983536	1636323	64.87%	7.901%
76	10.829	2949	2951	2954	rVB2	1049	578	0.02%	0.003%

LSC Area Percent Report

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Acq On : 02 May 2022 17:31
Operator : SY/MD
Sample : N2638-08
Misc : 5.36g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL03

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\SFAMULM042522WMA.M
Title : VOC Analysis

77	10.851	2954	2958	2959	rBV2	792	505	0.02%	0.002%
78	10.915	2976	2978	2981	rBV3	623	418	0.02%	0.002%
79	10.967	2992	2994	2998	rBV3	535	398	0.02%	0.002%
80	11.057	3013	3022	3029	rBV3	27730	41414	1.64%	0.200%
81	11.115	3030	3040	3057	rVB	383523	554779	21.99%	2.679%
82	11.311	3098	3101	3109	rVB4	2461	2471	0.10%	0.012%
83	11.578	3174	3184	3189	rBV6	3867	6683	0.26%	0.032%
84	11.639	3197	3203	3211	rBV8	1577	2499	0.10%	0.012%
85	11.687	3214	3218	3221	rBV4	1896	1932	0.08%	0.009%
86	11.816	3246	3258	3271	rBV	818154	1302867	51.65%	6.291%
87	11.874	3272	3276	3281	rVV3	14022	16934	0.67%	0.082%
88	11.912	3282	3288	3299	rVB3	21111	29695	1.18%	0.143%
89	12.002	3310	3316	3327	rVB2	20347	28563	1.13%	0.138%
90	12.198	3360	3377	3395	rBV	1249154	2008825	79.64%	9.699%
91	12.327	3408	3417	3429	rVB	80541	113267	4.49%	0.547%
92	12.481	3463	3465	3469	rBV4	579	470	0.02%	0.002%
93	13.140	3668	3670	3674	rBV	841	716	0.03%	0.003%
94	13.391	3738	3748	3755	rBV2	36437	52452	2.08%	0.253%
95	13.558	3798	3800	3802	rBV	736	485	0.02%	0.002%
96	13.587	3804	3809	3816	rVB3	3354	4353	0.17%	0.021%
97	14.092	3961	3966	3967	rBV3	1540	1334	0.05%	0.006%
98	14.449	4069	4077	4087	rBV3	10011	13387	0.53%	0.065%
99	14.816	4188	4191	4194	rBV4	759	568	0.02%	0.003%
100	15.375	4357	4365	4370	rBV7	9168	14682	0.58%	0.071%

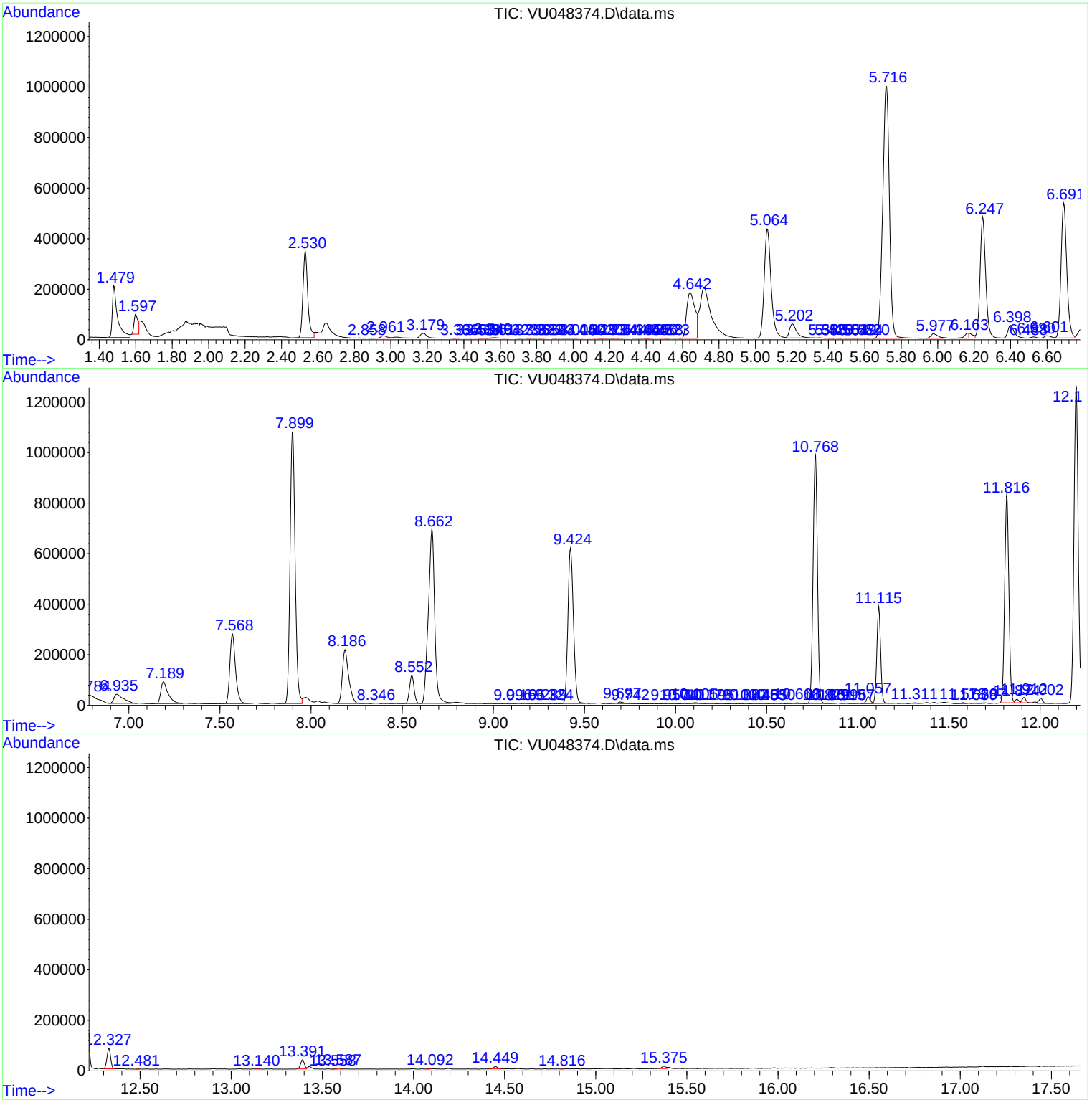
Sum of corrected areas: 20711606

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050222\
Data File : VU048374.D
Acq On : 02 May 2022 17:31
Operator : SY/MD
Sample : N2638-08
Misc : 5.36g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL03

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050222\
Data File : VU048374.D
Acq On : 02 May 2022 17:31
Operator : SY/MD
Sample : N2638-08
Misc : 5.36g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL03

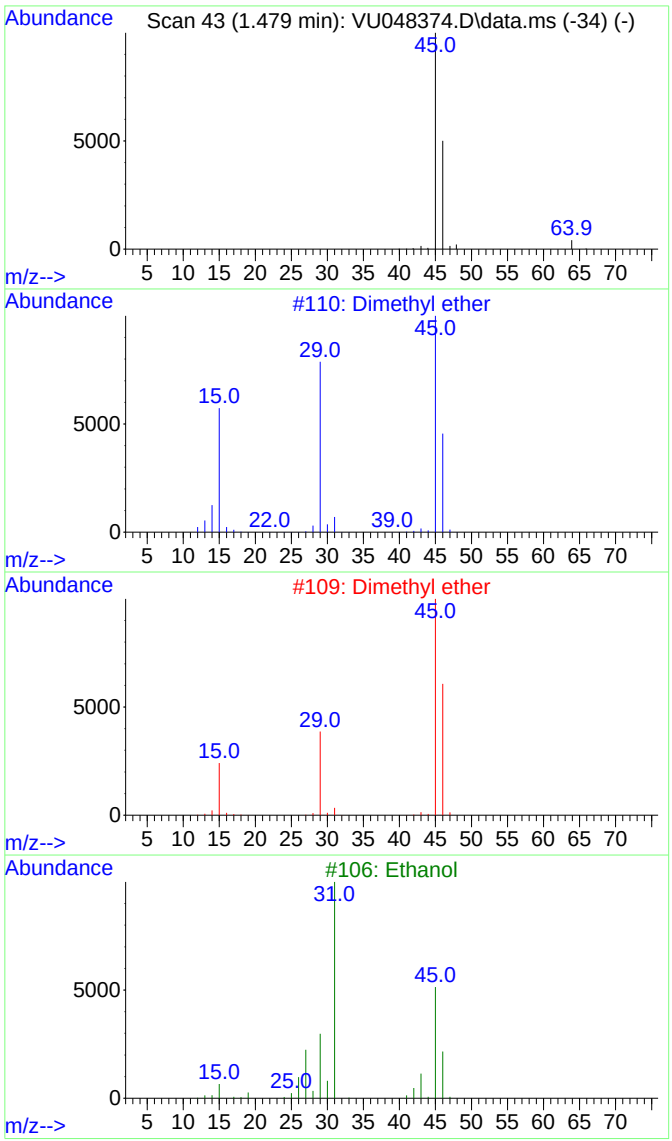
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

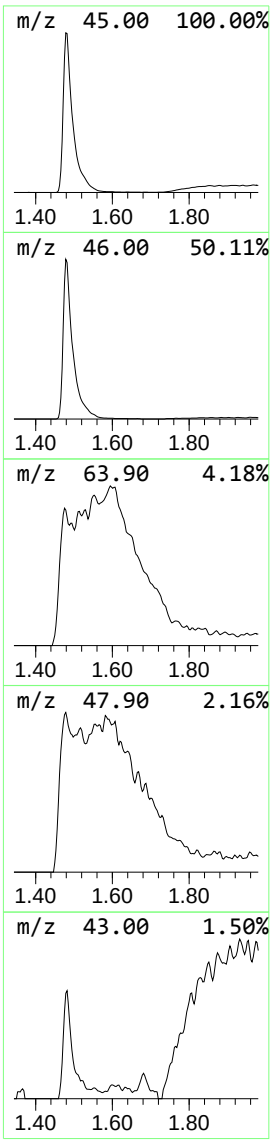
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Dimethyl ether Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.479	19.54 ug/L	402338	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl ether	46	C2H6O	000115-10-6	86
2	Dimethyl ether	46	C2H6O	000115-10-6	64
3	Ethanol	46	C2H6O	000064-17-5	7
4	Formic acid	46	CH2O2	000064-18-6	7
5	Ethanol	46	C2H6O	000064-17-5	7





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050222\
Data File : VU048374.D
Acq On : 02 May 2022 17:31
Operator : SY/MD
Sample : N2638-08
Misc : 5.36g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL03

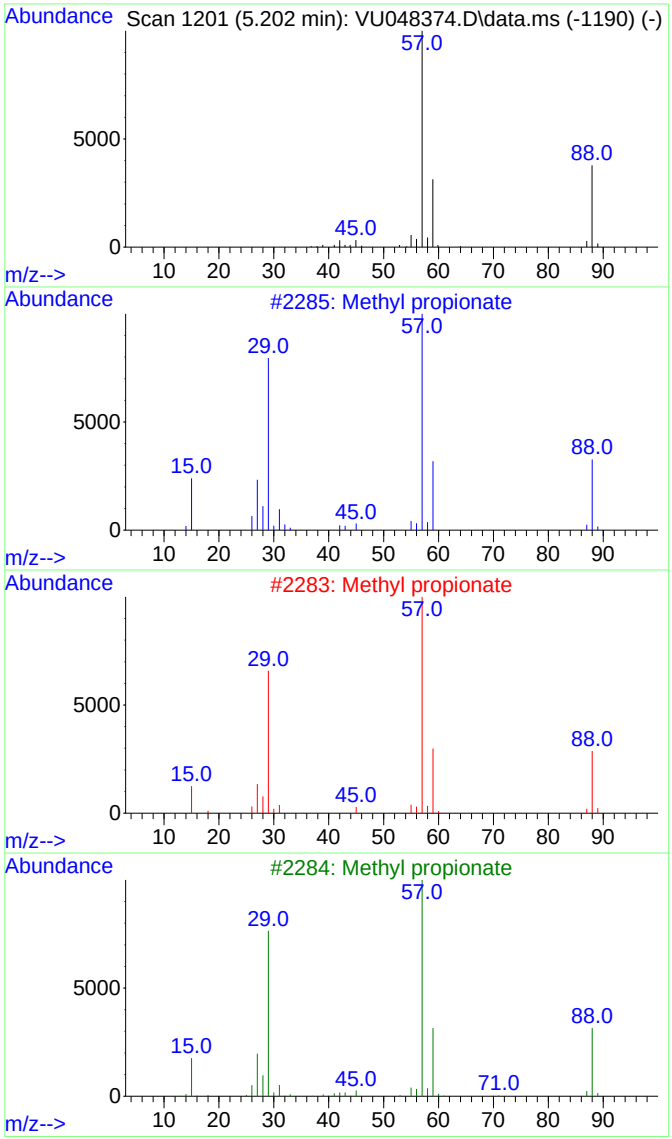
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

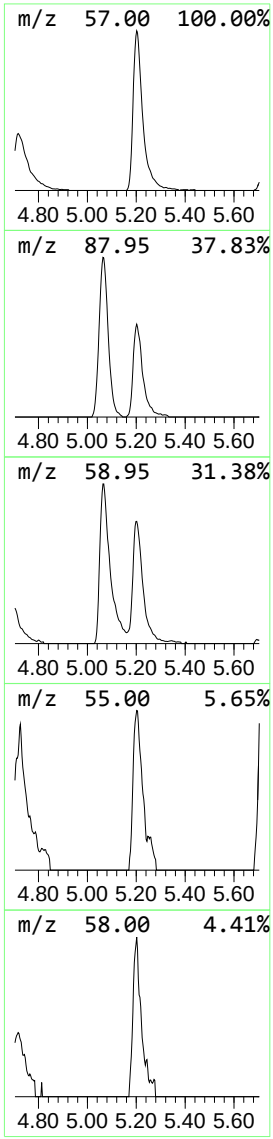
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Methyl propionate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.202	7.16 ug/L	147411	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	64
5	Methyl propionate	88	C4H8O2	000554-12-1	56





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050222\
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Acq On : 02 May 2022 17:31
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL03

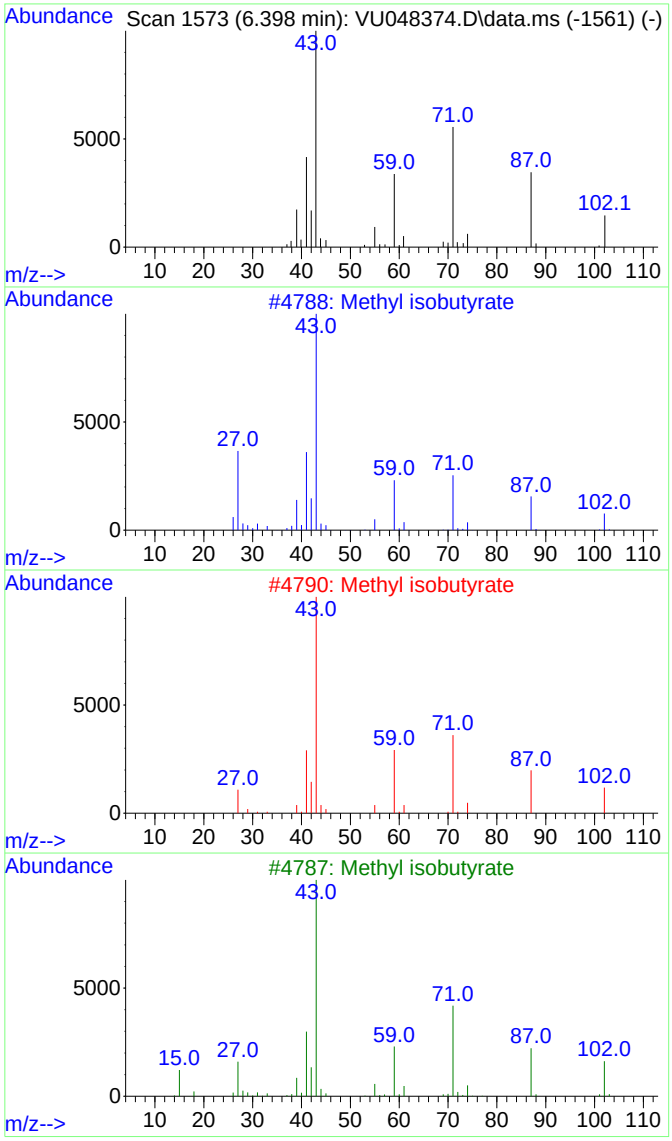
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

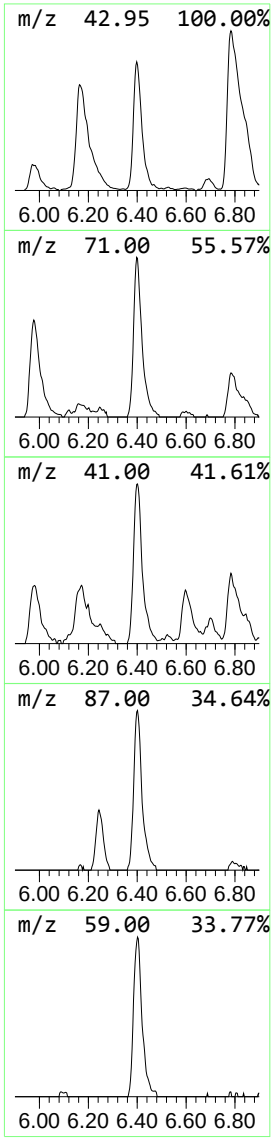
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Methyl isobutyrate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.398	5.99 ug/L	123262	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	91
3	Methyl isobutyrate	102	C5H10O2	000547-63-7	90
4	Methyl isobutyrate	102	C5H10O2	000547-63-7	64
5	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050222\
Data File : VU048374.D
Acq On : 02 May 2022 17:31
Operator : SY/MD
Sample : N2638-08
Misc : 5.36g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL03

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

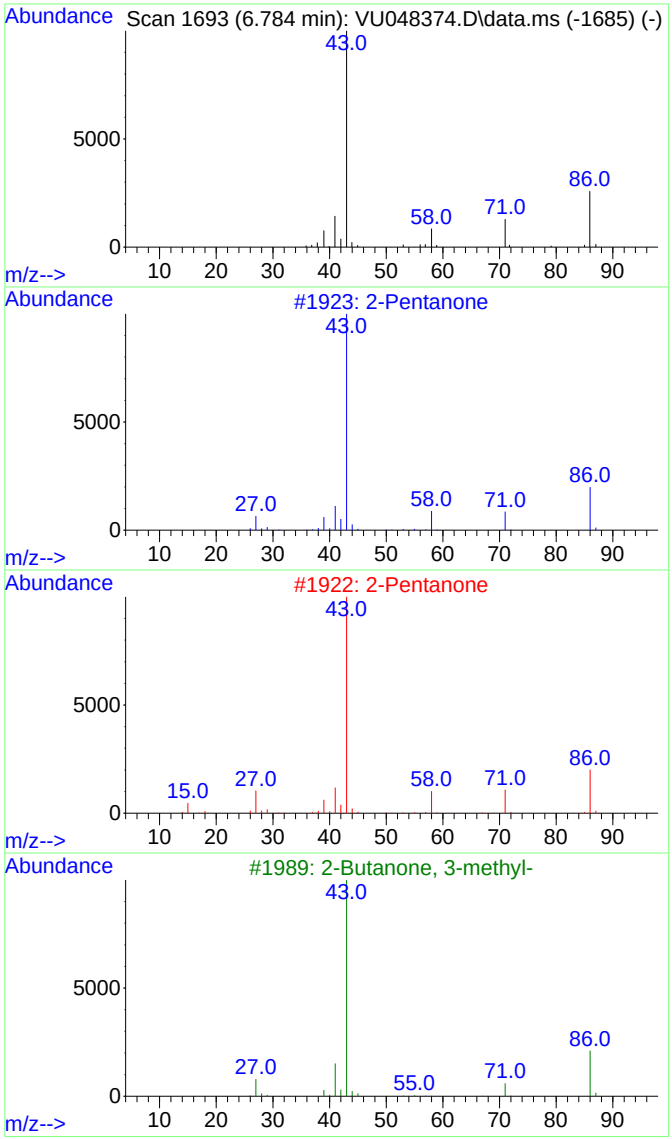
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

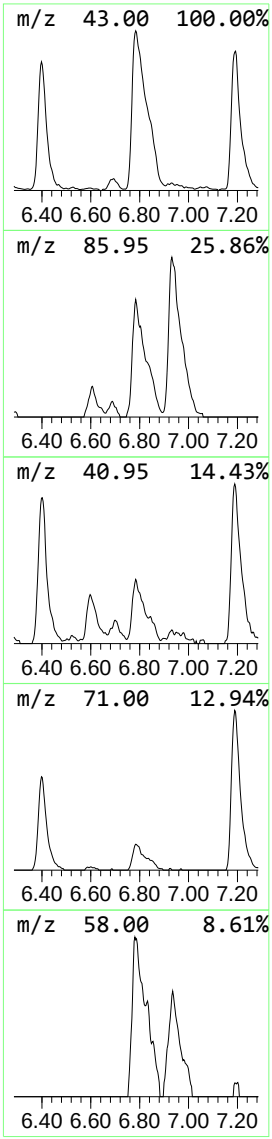
****

Peak Number 4 2-Pentanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.784	6.40 ug/L	131724	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	72
2	2-Pentanone	86	C5H10O	000107-87-9	64
3	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	59
4	2-Pentanone	86	C5H10O	000107-87-9	45
5	2,3-Hexanedione	114	C6H10O2	003848-24-6	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050222\
Data File : VU048374.D
Acq On : 02 May 2022 17:31
Operator : SY/MD
Sample : N2638-08
Misc : 5.36g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL03

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

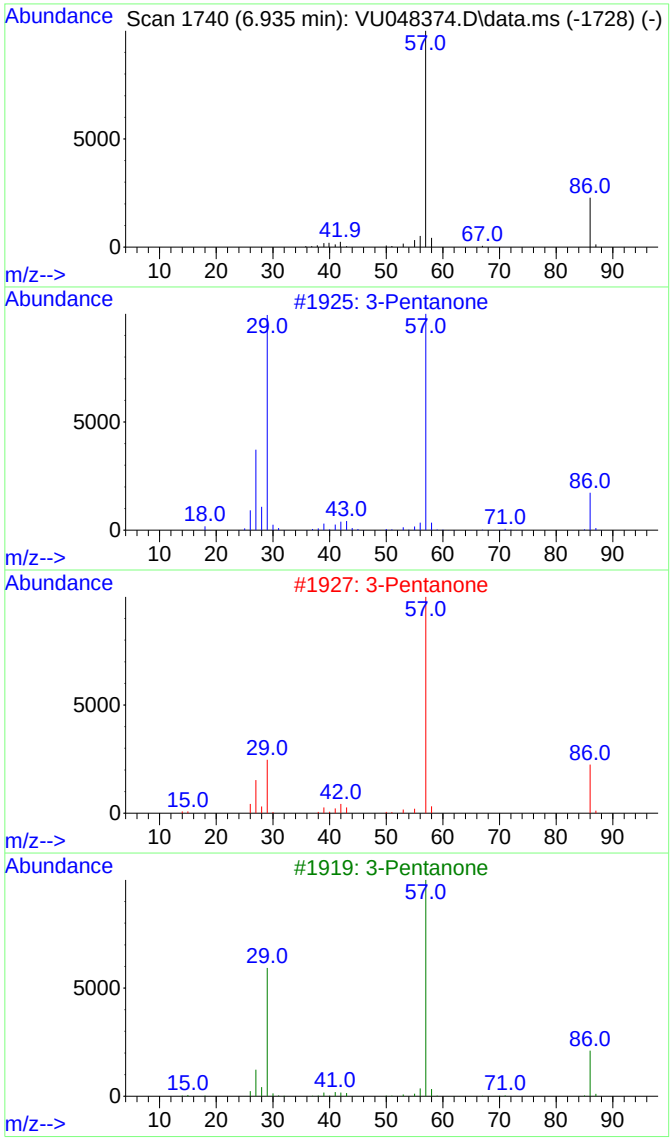
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

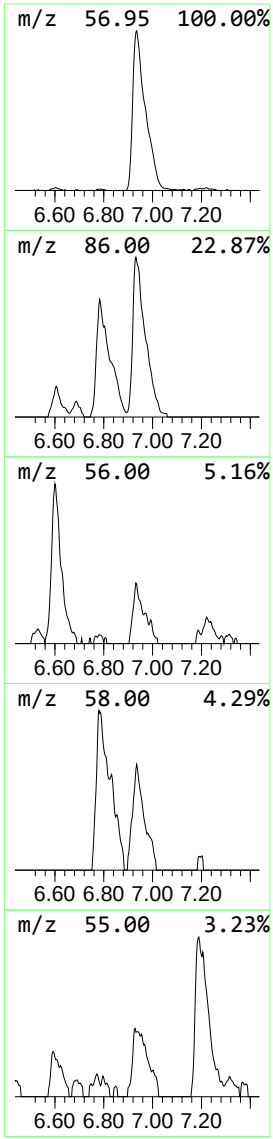
****

Peak Number 5 3-Pentanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.935	6.32 ug/L	130112	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	72
3	3-Pentanone	86	C5H10O	000096-22-0	72
4	Neopentane	72	C5H12	000463-82-1	28
5	3-Pentanone	86	C5H10O	000096-22-0	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050222\
Data File : VU048374.D
Acq On : 02 May 2022 17:31
Operator : SY/MD
Sample : N2638-08
Misc : 5.36g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL03

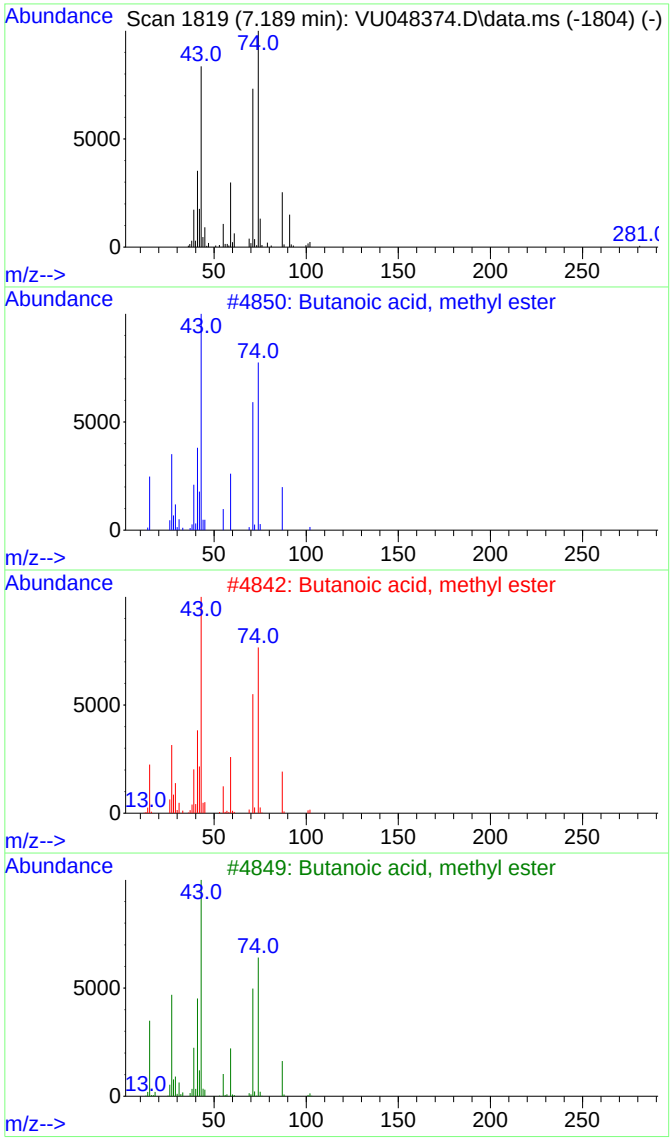
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

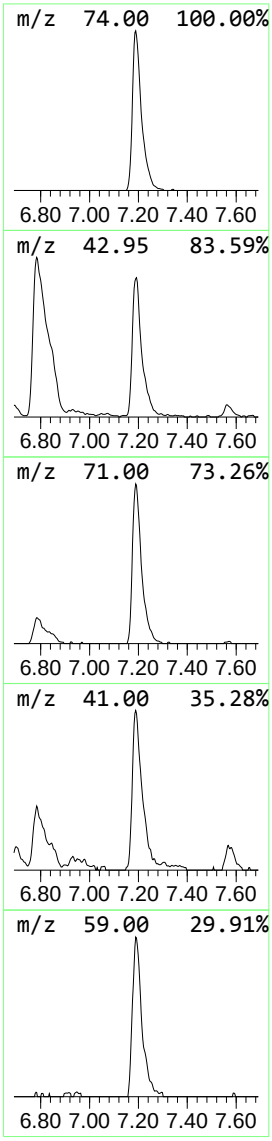
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Butanoic acid, methyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.189	11.91 ug/L	245162	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	87
3	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	83
4	Methyl isobutyrate	102	C5H10O2	000547-63-7	37
5	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050222\
Data File : VU048374.D
Acq On : 02 May 2022 17:31
Operator : SY/MD
Sample : N2638-08
Misc : 5.36g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL03

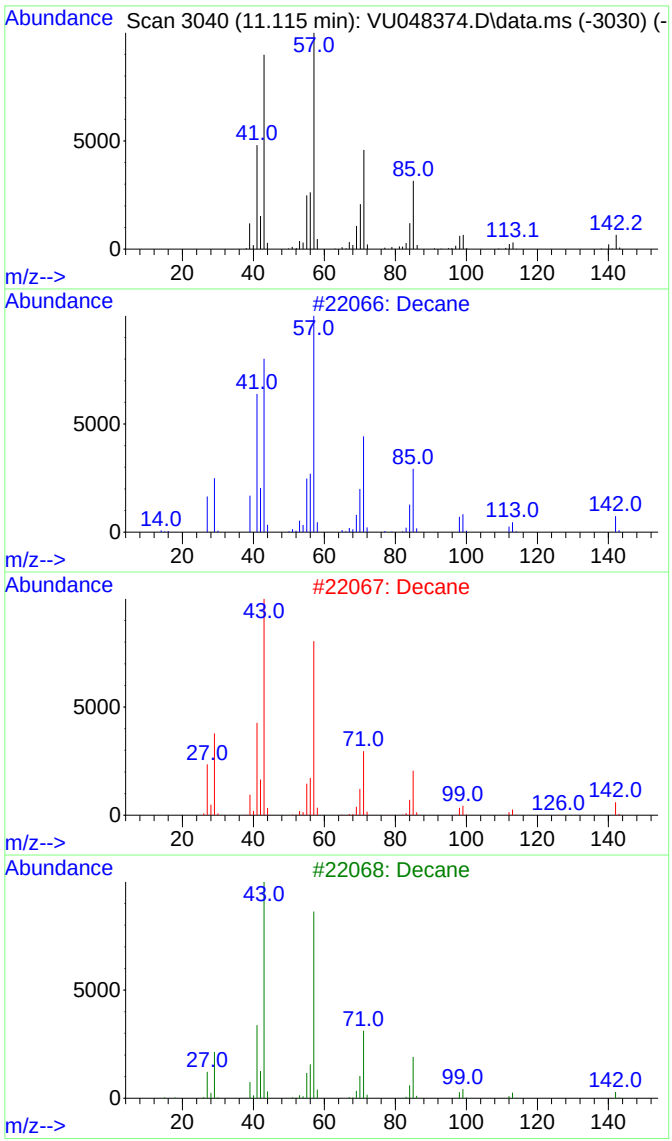
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

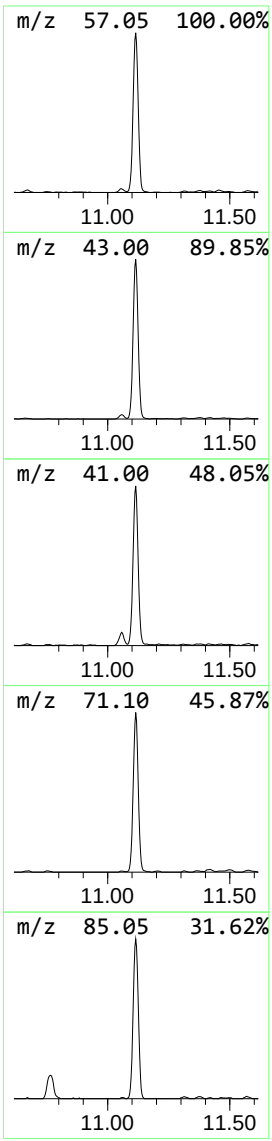
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.115	21.29 ug/L	554779	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	93
3	Decane	142	C10H22	000124-18-5	87
4	Decane	142	C10H22	000124-18-5	87
5	Carbonic acid, dodecyl prop-1-en...	270	C16H30O3	1000382-90-7	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050222\
Data File : VU048374.D
Acq On : 02 May 2022 17:31
Operator : SY/MD
Sample : N2638-08
Misc : 5.36g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL03

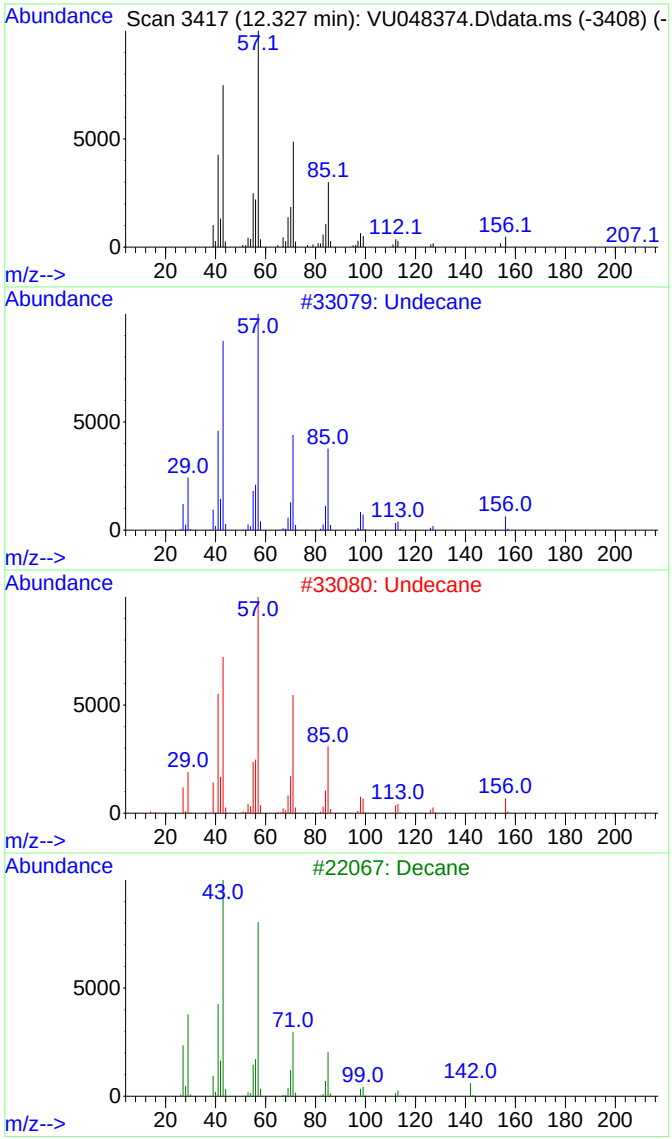
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

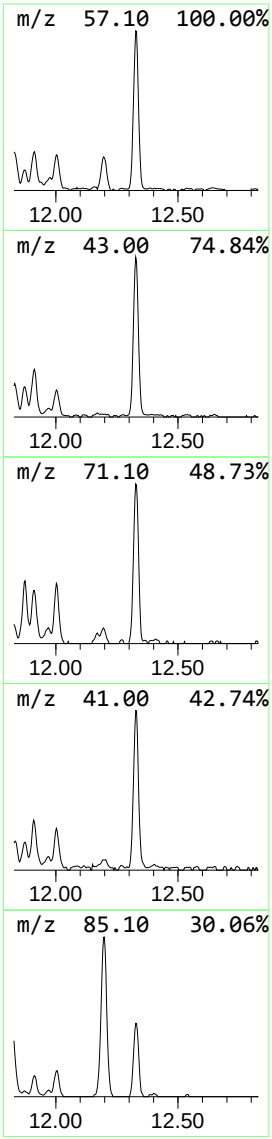
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.327	4.35 ug/L	113267	1,4-Dichlorobenzene-d4	11.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	93
2	Undecane	156	C11H24	001120-21-4	93
3	Decane	142	C10H22	000124-18-5	90
4	Undecane	156	C11H24	001120-21-4	87
5	Hexadecane	226	C16H34	000544-76-3	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050222\
Data File : VU048374.D
Acq On : 02 May 2022 17:31
Operator : SY/MD
Sample : N2638-08
Misc : 5.36g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL03

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.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	1.479	19.5	ug/L	402338	1	6.247	1029480	50.0
Methyl propionate	5.202	7.2	ug/L	147411	1	6.247	1029480	50.0
Methyl isobutyrate	6.398	6.0	ug/L	123262	1	6.247	1029480	50.0
2-Pentanone	6.784	6.4	ug/L	131724	1	6.247	1029480	50.0
3-Pentanone	6.935	6.3	ug/L	130112	1	6.247	1029480	50.0
Butanoic acid, ...	7.189	11.9	ug/L	245162	1	6.247	1029480	50.0
(DEL) Alkane: S...	11.115	21.3	ug/L	554779	3	11.816	1302870	50.0
(DEL) Alkane: S...	12.327	4.3	ug/L	113267	3	11.816	1302870	50.0