LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052522\
Data File : VU048665.D
Acq On : 25 May 2022 12:53
Operator : SY/MD
Sample : N2926-10ME
Misc : 3.17g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY19ME

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: VU048665.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	62	rVB	81748	99734	8.25%	1.067%
2	1.597	72	80	99	rBV	36950	59120	4.89%	0.632%
3	1.678	103	105	110	rVB4	1049	834	0.07%	0.009%
4	1.710	110	115	119	rBV2	405	417	0.03%	0.004%
5	1.781	126	137	138	rBV6	6340	8237	0.68%	0.088%
6	1.874	161	166	172	rBV	28837	33276	2.75%	0.356%
7	2.057	220	223	227	rBV3	405	363	0.03%	0.004%
8	2.138	245	248	250	rBV	456	322	0.03%	0.003%
9	2.150	250	252	257	rVB2	805	537	0.04%	0.006%
10	2.183	257	262	263	rBV	525	473	0.04%	0.005%
11	2.208	267	270	273	rVB3	517	343	0.03%	0.004%
12	2.253	281	284	287	rVB2	889	571	0.05%	0.006%
13	2.292	287	296	301	rBV3	1557	2421	0.20%	0.026%
14	2.334	306	309	310	rBV3	827	496	0.04%	0.005%
15	2.363	313	318	327	rBV	5051	8264	0.68%	0.088%
16	2.430	334	339	345	rBV4	3791	4780	0.40%	0.051%
17	2.536	362	372	384	rVB	193433	293294	24.26%	3.138%
18	2.636	394	403	419	rVB3	26972	49514	4.10%	0.530%
19	2.732	431	433	437	rVB3	570	329	0.03%	0.004%
20	2.758	438	441	445	rVB3	1062	764	0.06%	0.008%
21	2.829	459	463	467	rBV2	550	488	0.04%	0.005%
22	2.880	476	479	484	rVB2	590	398	0.03%	0.004%
23	2.948	490	500	516	rBV2	12801	24499	2.03%	0.262%
24	3.031	521	526	534	rVB4	1891	2434	0.20%	0.026%
25	3.182	552	573	585	rBV	14507	36133	2.99%	0.387%
26	3.260	593	597	602	rVB2	828	828	0.07%	0.009%
27	3.446	651	655	658	rBV2	344	298	0.02%	0.003%
28	3.568	683	693	694	rBV4	1578	1941	0.16%	0.021%
29	3.684	725	729	732	rBV2	534	417	0.03%	0.004%
30	3.739	742	746	752	rBV2	560	576	0.05%	0.006%
31	3.819	764	771	777	rBV2	514	709	0.06%	0.008%
32	4.025	831	835	838	rBV	643	515	0.04%	0.006%
33	4.054	838	844	850	rBV4	783	1165	0.10%	0.012%
34	4.134	866	869	876	rVB2	308	325	0.03%	0.003%
35	4.179	880	883	886	rVV	453	354	0.03%	0.004%
36	4.208	889	892	896	rVB	828	598	0.05%	0.006%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052522\
Data File : VU048665.D
Acq On : 25 May 2022 12:53
Operator : SY/MD
Sample : N2926-10ME
Misc : 3.17g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY19ME

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	4.253	901	906	908	rBV2	349	347	0.03%	0.004%
38	4.330	928	930	934	rVB	594	317	0.03%	0.003%
39	4.350	934	936	940	rBV	685	414	0.03%	0.004%
40	4.469	969	973	977	rBV2	432	473	0.04%	0.005%
41	4.629	1005	1023	1037	rBV	63542	177383	14.67%	1.898%
42	4.922	1110	1114	1119	rVB3	769	691	0.06%	0.007%
43	5.060	1141	1157	1180	rBV	153219	362087	29.95%	3.874%
44	5.198	1189	1200	1220	rVB2	24936	54496	4.51%	0.583%
45	5.343	1236	1245	1247	rBV2	973	1252	0.10%	0.013%
46	5.388	1256	1259	1263	rVB2	809	643	0.05%	0.007%
47	5.424	1263	1270	1272	rBV	528	559	0.05%	0.006%
48	5.469	1281	1284	1289	rVB2	534	421	0.03%	0.005%
49	5.597	1320	1324	1326	rBV	566	397	0.03%	0.004%
50	5.716	1341	1361	1385	rVV2	262280	699458	57.86%	7.483%
51	5.825	1393	1395	1400	rVB	713	519	0.04%	0.006%
52	5.851	1400	1403	1405	rBV	578	374	0.03%	0.004%
53	5.970	1429	1440	1445	rBV6	7192	12552	1.04%	0.134%
54	6.157	1487	1498	1513	rBV2	8385	23026	1.90%	0.246%
55	6.247	1513	1526	1555	rVB	268344	537199	44.43%	5.747%
56	6.398	1562	1573	1596	rVB4	23332	52539	4.35%	0.562%
57	6.523	1604	1612	1621	rVB5	4829	7925	0.66%	0.085%
58	6.594	1625	1634	1643	rBV5	3702	7050	0.58%	0.075%
59	6.690	1650	1664	1681	rBV2	155339	316890	26.21%	3.390%
60	6.780	1681	1692	1704	rBV2	13878	34952	2.89%	0.374%
61	6.925	1726	1737	1770	rVB	16160	50411	4.17%	0.539%
62	7.057	1774	1778	1780	rBV2	523	389	0.03%	0.004%
63	7.102	1789	1792	1795	rBV	598	439	0.04%	0.005%
64	7.186	1808	1818	1841	rBV4	42103	98863	8.18%	1.058%
65	7.295	1849	1852	1857	rVB3	818	620	0.05%	0.007%
66	7.378	1869	1878	1888	rBV4	1710	2742	0.23%	0.029%
67	7.565	1924	1936	1958	rVB2	90806	176026	14.56%	1.883%
68	7.658	1961	1965	1970	rVB2	629	478	0.04%	0.005%
69	7.690	1970	1975	1982	rBV4	1555	2059	0.17%	0.022%
70	7.768	1994	1999	2000	rBV	787	615	0.05%	0.007%
71	7.787	2000	2005	2006	rBV2	1645	1249	0.10%	0.013%
72	7.896	2026	2039	2054	rBV	309039	548819	45.40%	5.871%
73	8.034	2078	2082	2091	rBV5	2507	2938	0.24%	0.031%
74	8.182	2117	2128	2151	rVB2	80478	172084	14.23%	1.841%
75	8.324	2168	2172	2175	rVB2	490	374	0.03%	0.004%
76	8.369	2184	2186	2191	rVB2	537	411	0.03%	0.004%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052522\
Data File : VU048665.D
Acq On : 25 May 2022 12:53
Operator : SY/MD
Sample : N2926-10ME
Misc : 3.17g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY19ME

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	8.478	2216	2220	2225	rBV2	507	476	0.04%	0.005%
78	8.552	2230	2243	2256	rBV4	19053	32969	2.73%	0.353%
79	8.652	2256	2274	2302	rVV	230330	513642	42.49%	5.495%
80	8.784	2311	2315	2317	rBV3	1276	1065	0.09%	0.011%
81	8.857	2333	2338	2342	rBV3	1113	1208	0.10%	0.013%
82	8.919	2354	2357	2363	rVB5	2078	2177	0.18%	0.023%
83	9.005	2379	2384	2389	rBV2	1966	2236	0.18%	0.024%
84	9.150	2423	2429	2434	rBV	2719	3905	0.32%	0.042%
85	9.420	2501	2513	2531	rBV	565183	1080083	89.34%	11.555%
86	10.764	2919	2931	2951	rVB	494186	814894	67.40%	8.718%
87	11.060	3014	3023	3030	rBV4	23834	35723	2.95%	0.382%
88	11.115	3030	3040	3060	rVB	317708	476946	39.45%	5.102%
89	11.816	3246	3258	3271	rBV	751430	1208959	100.00%	12.933%
90	12.005	3310	3317	3327	rVB4	16734	24412	2.02%	0.261%
91	12.195	3364	3376	3395	rBV	614733	1012087	83.72%	10.827%
92	12.327	3409	3417	3431	rVB	58919	81785	6.76%	0.875%
93	13.391	3739	3748	3756	rBV2	30590	44536	3.68%	0.476%
94	14.095	3960	3967	3977	rVB3	7833	12949	1.07%	0.139%
95	15.372	4359	4364	4370	rBV7	6046	6098	0.50%	0.065%
96	15.478	4393	4397	4399	rBV	716	502	0.04%	0.005%
97	15.713	4466	4470	4471	rBV	725	511	0.04%	0.005%
98	15.758	4481	4484	4487	rVV2	731	471	0.04%	0.005%
99	16.262	4630	4641	4645	rBV9	1809	2858	0.24%	0.031%
100	16.330	4660	4662	4666	rVB2	2001	873	0.07%	0.009%

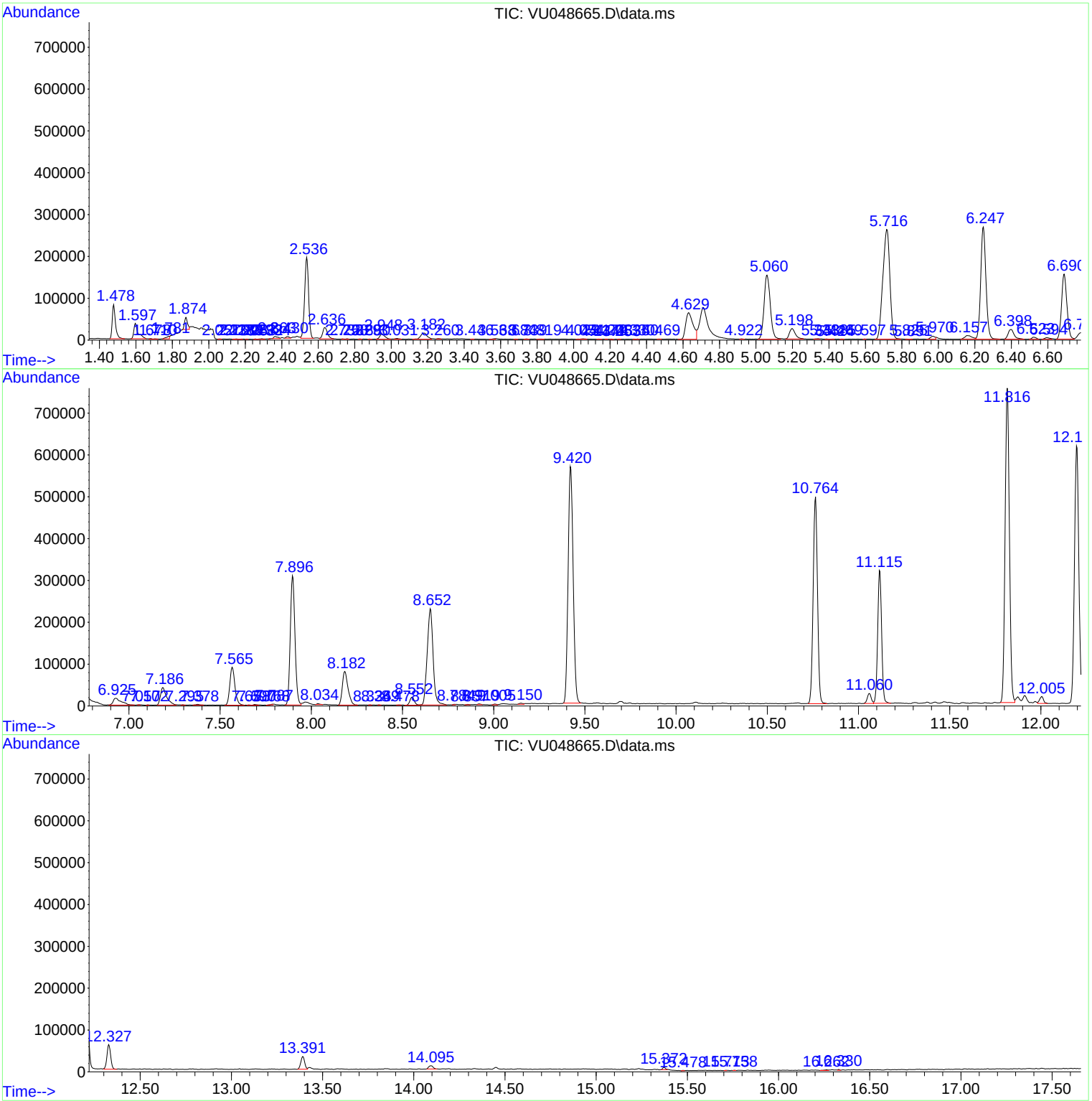
Sum of corrected areas: 9347613

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052522\
Data File : VU048665.D
Acq On : 25 May 2022 12:53
Operator : SY/MD
Sample : N2926-10ME
Misc : 3.17g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY19ME

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 : VU048665.D
Acq On : 25 May 2022 12:53
Operator : SY/MD
Sample : N2926-10ME
Misc : 3.17g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY19ME

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

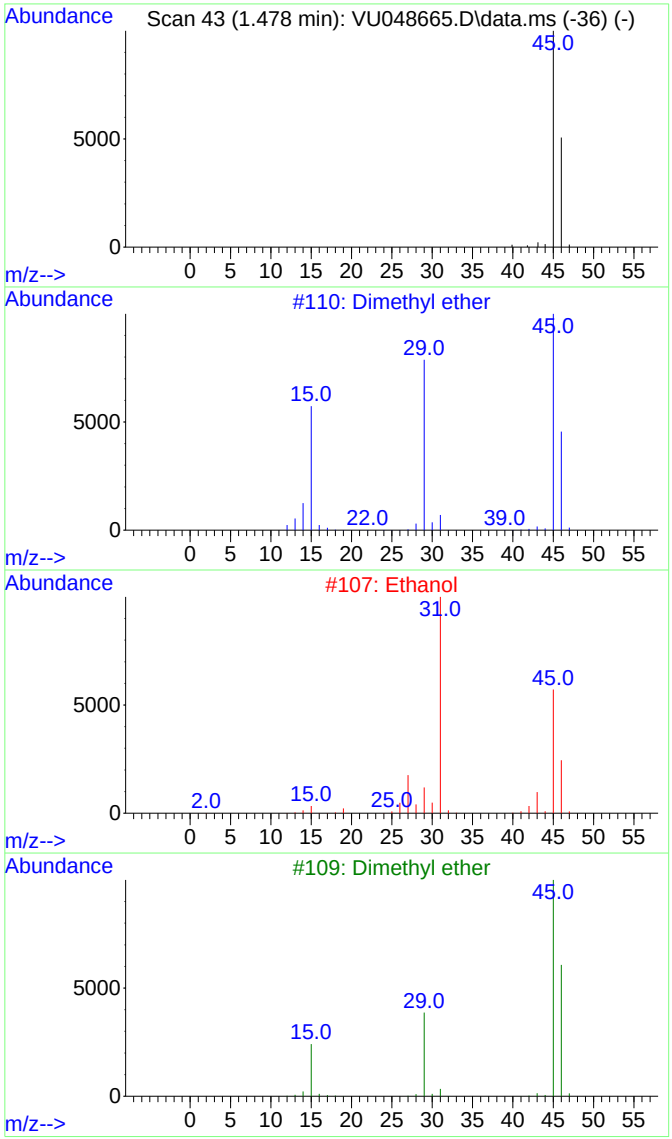
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

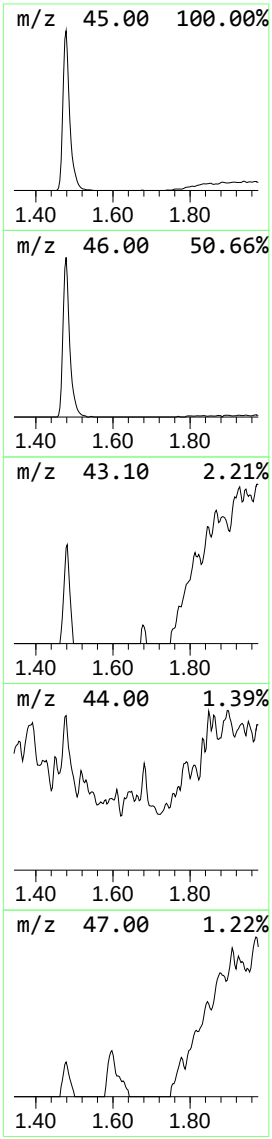
****

Peak Number 1 Dimethyl ether Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.478	9.28 ug/L	99734	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl ether	46	C2H6O	000115-10-6	83
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	7





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052522\
Data File : VU048665.D
Acq On : 25 May 2022 12:53
Operator : SY/MD
Sample : N2926-10ME
Misc : 3.17g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY19ME

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

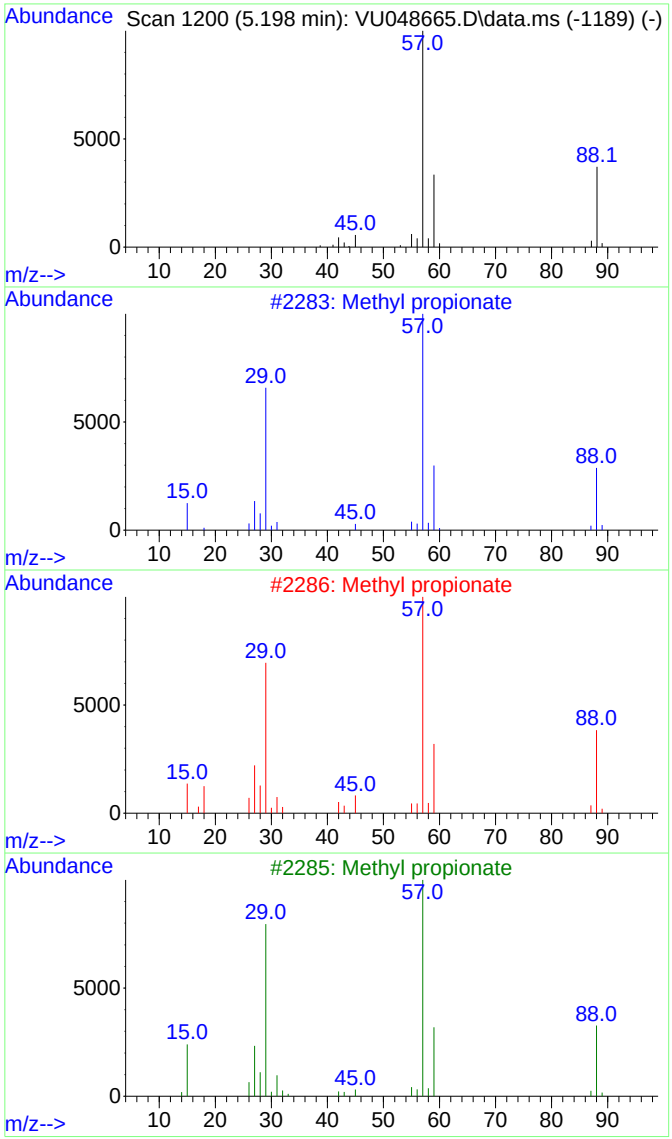
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

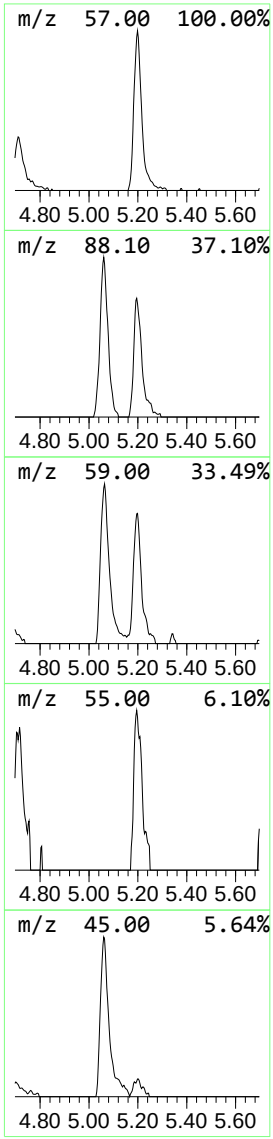
****

Peak Number 3 Methyl propionate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.198	5.07 ug/L	54496	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	90
3	Methyl propionate	88	C4H8O2	000554-12-1	86
4	Methyl propionate	88	C4H8O2	000554-12-1	80
5	Methyl propionate	88	C4H8O2	000554-12-1	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052522\
Data File : VU048665.D
Acq On : 25 May 2022 12:53
Operator : SY/MD
Sample : N2926-10ME
Misc : 3.17g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY19ME

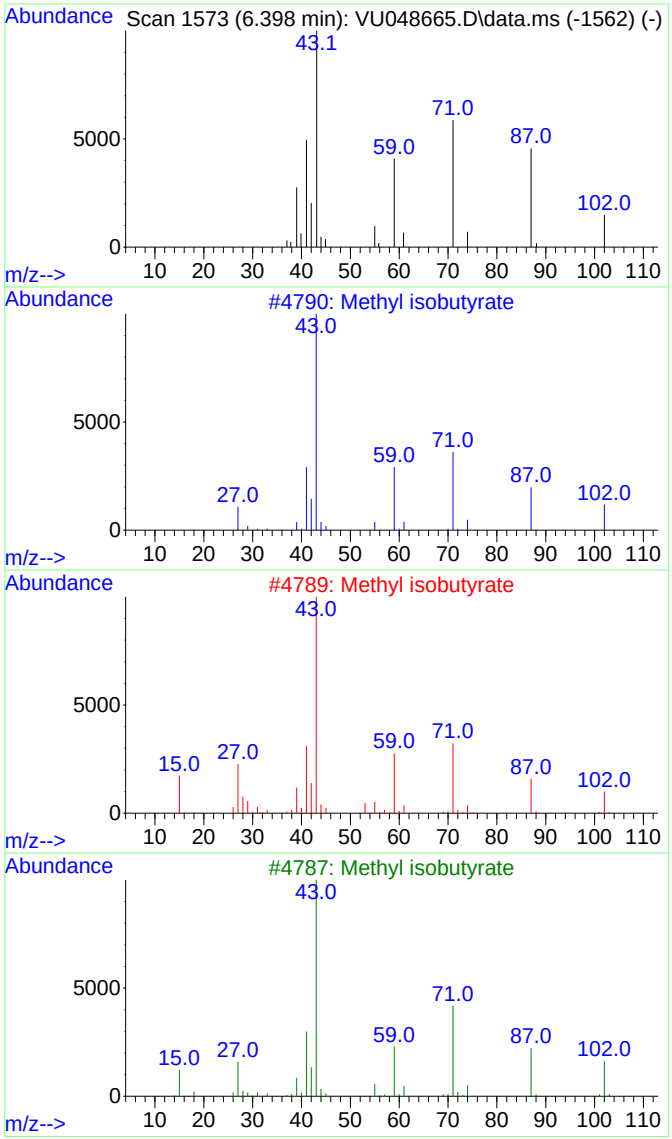
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

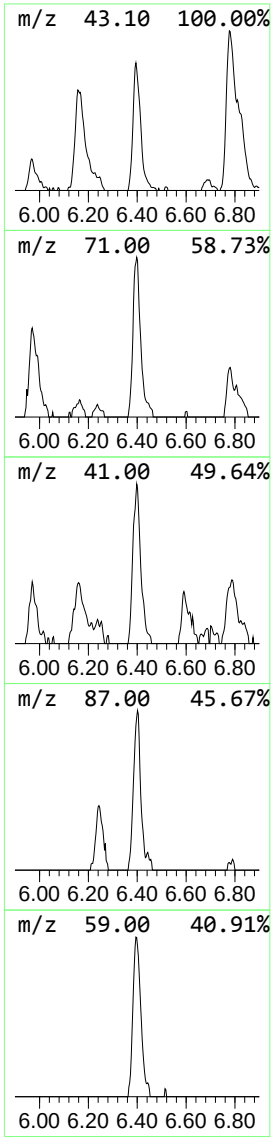
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.398	4.89 ug/L	52539	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl isobutyrate	102	C5H10O2	000547-63-7	68
2	Methyl isobutyrate	102	C5H10O2	000547-63-7	58
3	Methyl isobutyrate	102	C5H10O2	000547-63-7	53
4	Methyl isobutyrate	102	C5H10O2	000547-63-7	52
5	Cycloserine	102	C3H6N2O2	000068-41-7	17





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052522\
Data File : VU048665.D
Acq On : 25 May 2022 12:53
Operator : SY/MD
Sample : N2926-10ME
Misc : 3.17g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY19ME

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

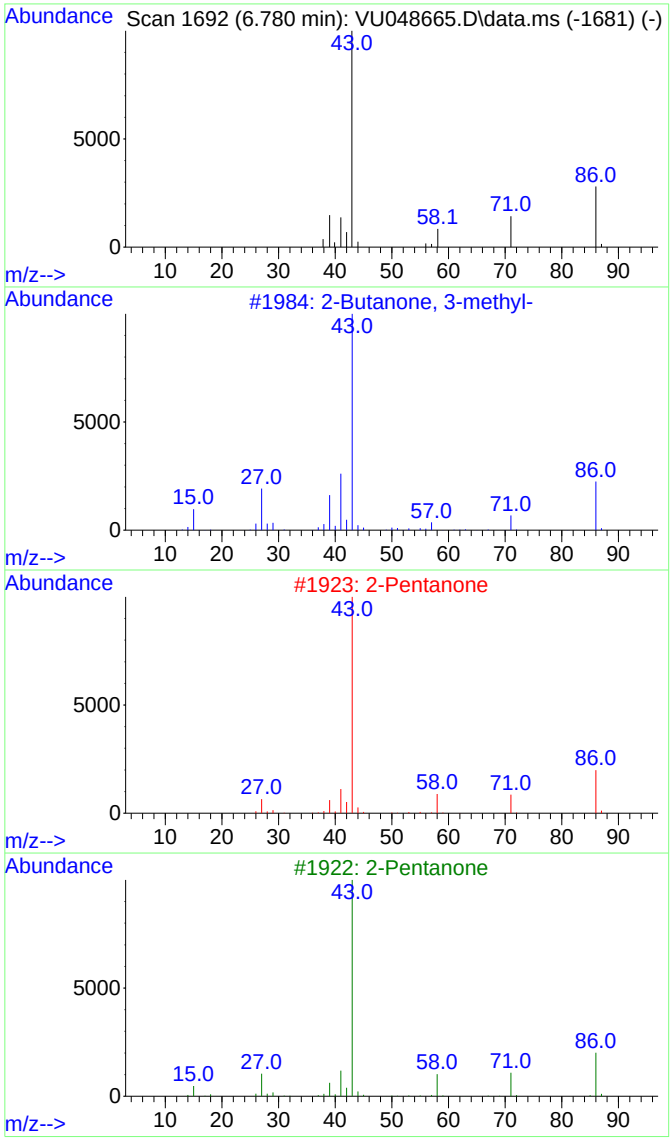
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

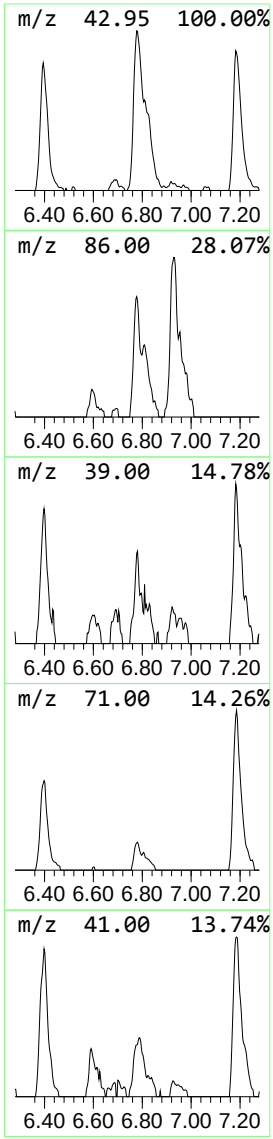
****

Peak Number 5 2-Butanone, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.780	3.25 ug/L	34952	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	80
2	2-Pentanone	86	C5H10O	000107-87-9	78
3	2-Pentanone	86	C5H10O	000107-87-9	72
4	2-Pentanone	86	C5H10O	000107-87-9	72
5	3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	36





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052522\
Data File : VU048665.D
Acq On : 25 May 2022 12:53
Operator : SY/MD
Sample : N2926-10ME
Misc : 3.17g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY19ME

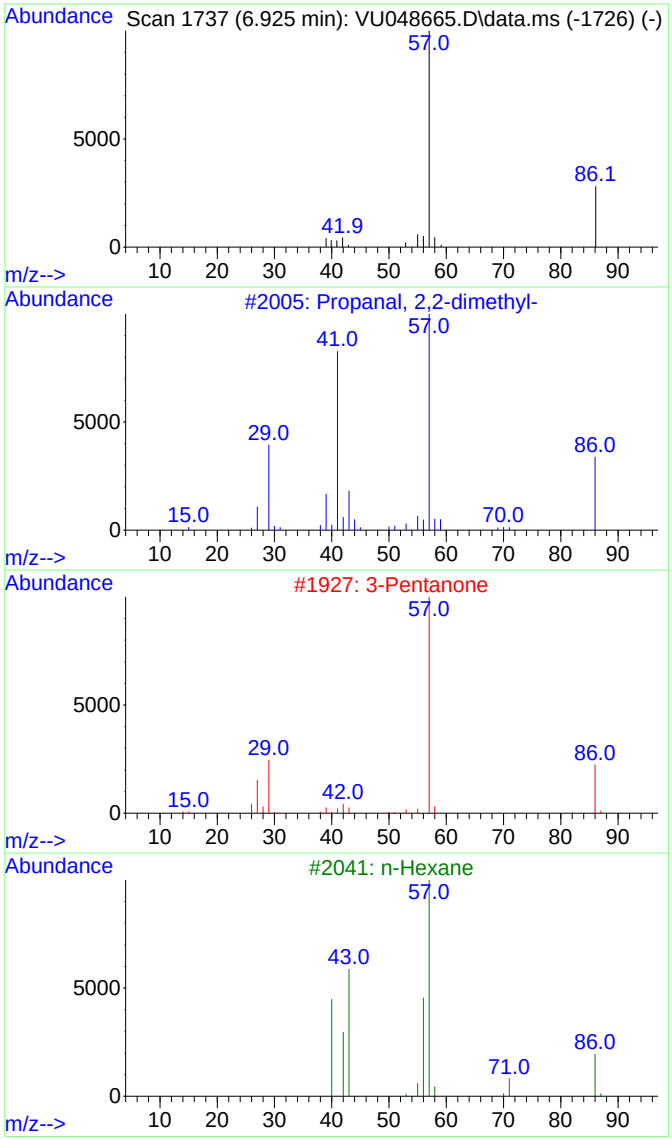
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

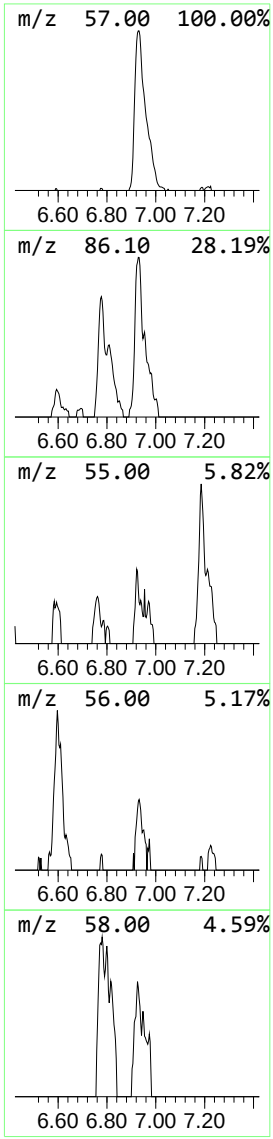
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Propanal, 2,2-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.925	4.69 ug/L	50411	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	78
2	3-Pentanone	86	C5H10O	000096-22-0	72
3	n-Hexane	86	C6H14	000110-54-3	39
4	3-Pentanone	86	C5H10O	000096-22-0	28
5	3-Pentanone	86	C5H10O	000096-22-0	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052522\
Data File : VU048665.D
Acq On : 25 May 2022 12:53
Operator : SY/MD
Sample : N2926-10ME
Misc : 3.17g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY19ME

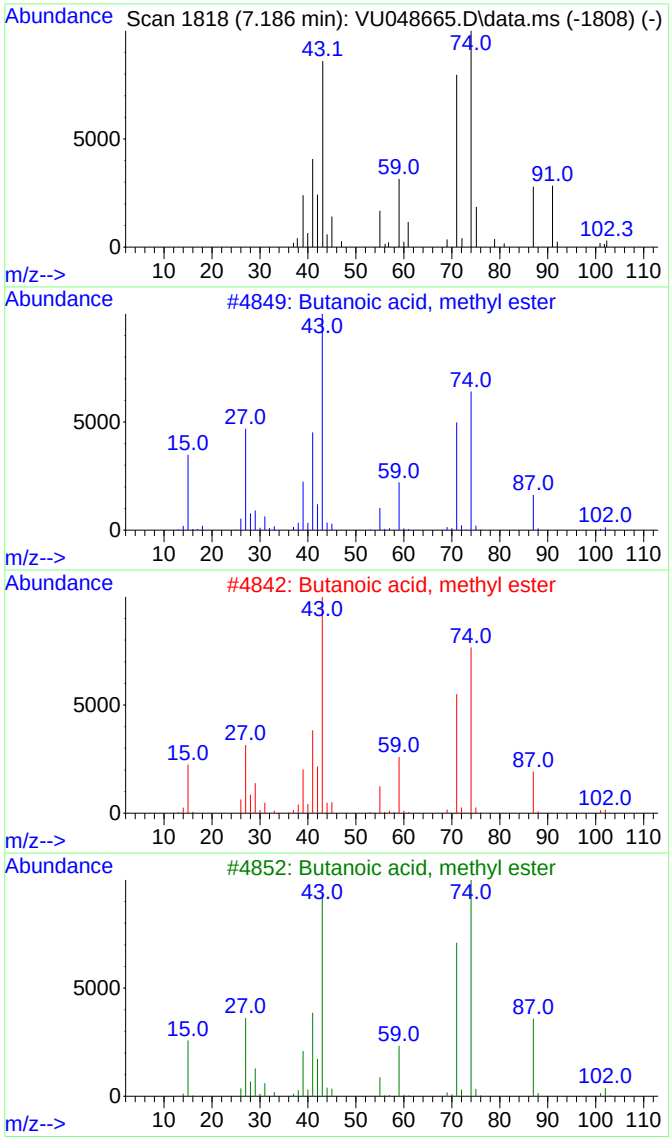
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

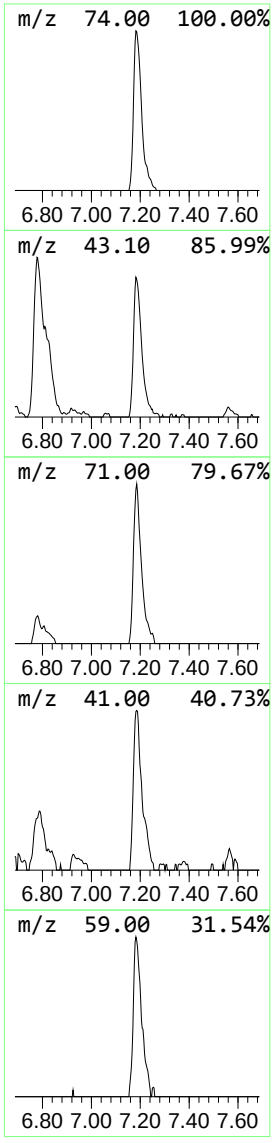
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Butanoic acid, methyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.186	9.20 ug/L	98863	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	80
2	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	78
3	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	72
4	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	72
5	Methyl isobutyrate	102	C5H10O2	000547-63-7	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052522\
Data File : VU048665.D
Acq On : 25 May 2022 12:53
Operator : SY/MD
Sample : N2926-10ME
Misc : 3.17g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY19ME

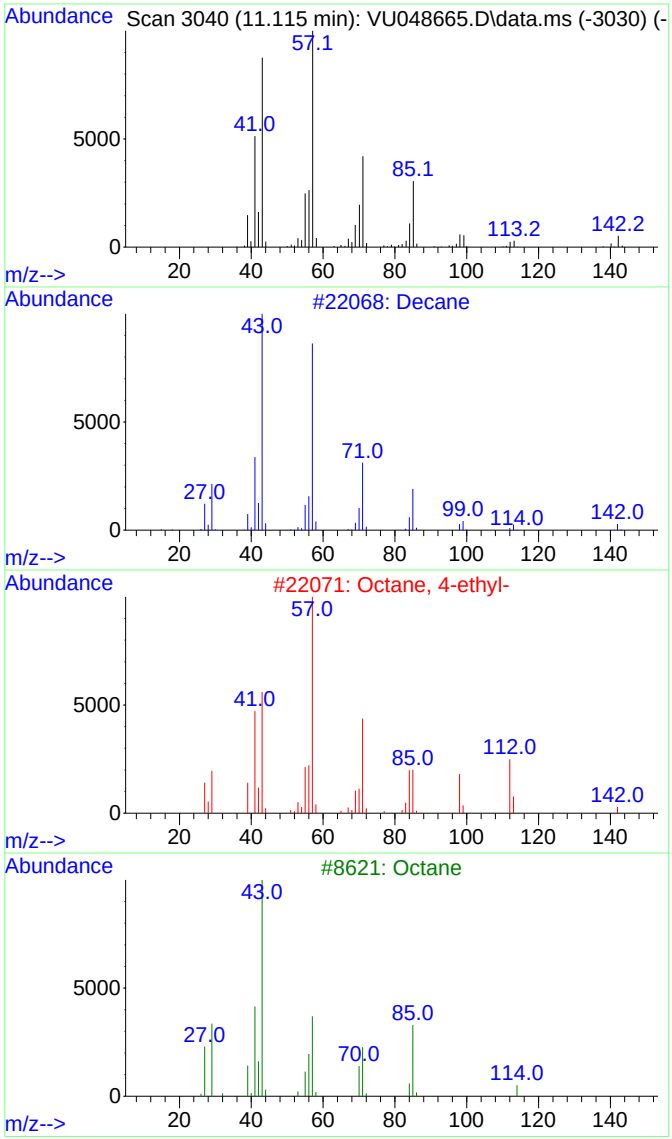
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

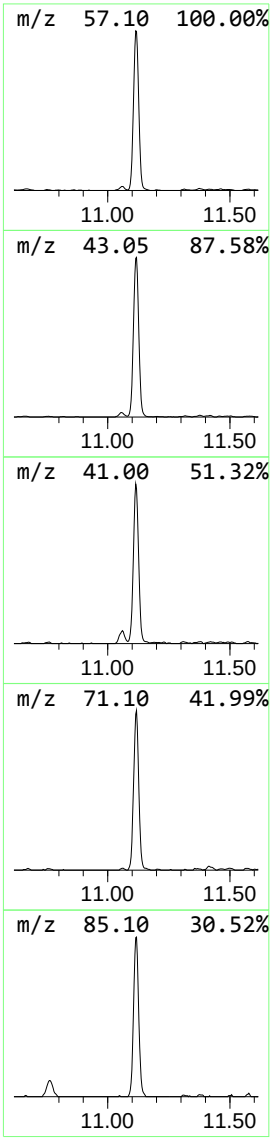
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.115	19.73 ug/L	476946	1,4-Dichlorobenzene-d4	11.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane	142	C10H22	000124-18-5	87
2	Octane, 4-ethyl-	142	C10H22	015869-86-0	72
3	Octane	114	C8H18	000111-65-9	64
4	Tridecane	184	C13H28	000629-50-5	53
5	Decane	142	C10H22	000124-18-5	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052522\
Data File : VU048665.D
Acq On : 25 May 2022 12:53
Operator : SY/MD
Sample : N2926-10ME
Misc : 3.17g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY19ME

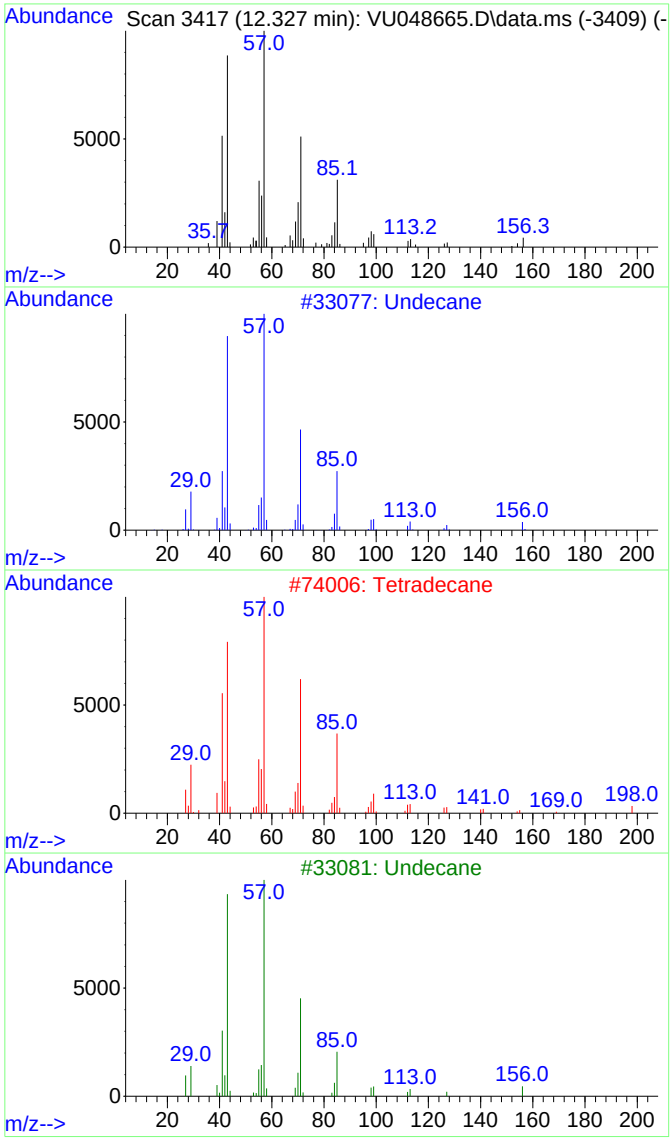
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

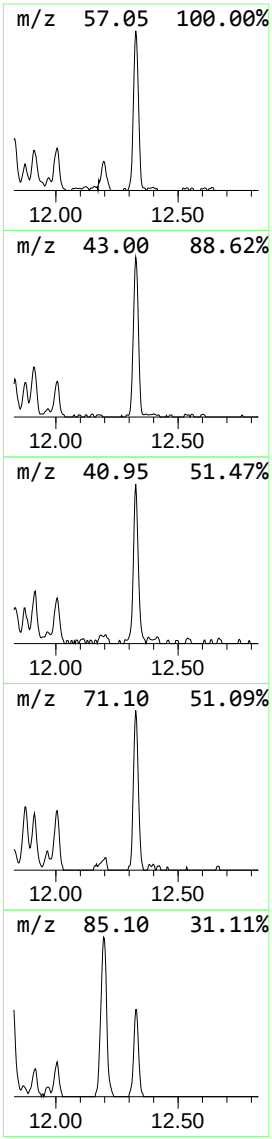
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.327	3.38 ug/L	81785	1,4-Dichlorobenzene-d4	11.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	87
2	Tetradecane	198	C14H30	000629-59-4	86
3	Undecane	156	C11H24	001120-21-4	83
4	Undecane	156	C11H24	001120-21-4	81
5	Undecane	156	C11H24	001120-21-4	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052522\
Data File : VU048665.D
Acq On : 25 May 2022 12:53
Operator : SY/MD
Sample : N2926-10ME
Misc : 3.17g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXY19ME

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	9.3	ug/L	99734	1	6.247	537199	50.0
Methyl propionate	5.198	5.1	ug/L	54496	1	6.247	537199	50.0
Methyl isobutyrate	6.398	4.9	ug/L	52539	1	6.247	537199	50.0
2-Butanone, 3-m...	6.780	3.3	ug/L	34952	1	6.247	537199	50.0
Propanal, 2,2-d...	6.925	4.7	ug/L	50411	1	6.247	537199	50.0
Butanoic acid, ...	7.186	9.2	ug/L	98863	1	6.247	537199	50.0
(DEL) Alkane: S...	11.115	19.7	ug/L	476946	3	11.816	1208960	50.0
(DEL) Alkane: S...	12.327	3.4	ug/L	81785	3	11.816	1208960	50.0