LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050422\
Data File : VU048413.D
Acq On : 04 May 2022 14:44
Operator : SY/MD
Sample : N2639-09
Misc : 5.86g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL19

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: VU048413.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.482	36	44	72	rBV	207870	366347	29.01%	2.794%
2	1.597	74	80	87	rBV	39353	59881	4.74%	0.457%
3	2.533	359	371	391	rBV	151596	294404	23.31%	2.245%
4	2.642	398	405	438	rVB4	45778	130452	10.33%	0.995%
5	2.877	475	478	480	rBV3	345	266	0.02%	0.002%
6	2.961	494	504	517	rBV	9190	20252	1.60%	0.154%
7	3.176	556	571	588	rBV	18917	44303	3.51%	0.338%
8	3.353	624	626	627	rBV2	472	212	0.02%	0.002%
9	3.568	684	693	712	rVB6	2926	7593	0.60%	0.058%
10	3.668	718	724	729	rBV4	567	694	0.05%	0.005%
11	3.858	774	783	787	rBV4	393	586	0.05%	0.004%
12	4.009	826	830	834	rBV3	345	317	0.03%	0.002%
13	4.041	838	840	842	rVV2	411	254	0.02%	0.002%
14	4.067	842	848	857	rVB4	840	1530	0.12%	0.012%
15	4.279	909	914	918	rBV2	192	231	0.02%	0.002%
16	4.301	918	921	923	rBV3	326	227	0.02%	0.002%
17	4.317	923	926	927	rBV	448	218	0.02%	0.002%
18	4.459	959	970	972	rBV3	623	793	0.06%	0.006%
19	4.555	993	1000	1007	rBV2	536	640	0.05%	0.005%
20	4.649	1011	1029	1041	rBV	95655	287957	22.80%	2.196%
21	5.063	1142	1158	1190	rBV2	249807	625617	49.54%	4.771%
22	5.205	1191	1202	1239	rVB	59322	151059	11.96%	1.152%
23	5.366	1249	1252	1256	rVB5	735	414	0.03%	0.003%
24	5.456	1277	1280	1282	rBV3	251	221	0.02%	0.002%
25	5.520	1296	1300	1304	rVB4	603	590	0.05%	0.004%
26	5.616	1325	1330	1332	rBV3	320	237	0.02%	0.002%
27	5.716	1341	1361	1389	rBV2	486641	1250091	98.99%	9.534%
28	5.980	1431	1443	1472	rBV2	16640	45364	3.59%	0.346%
29	6.115	1482	1485	1486	rBV2	876	459	0.04%	0.004%
30	6.169	1493	1502	1512	rBV2	13118	29753	2.36%	0.227%
31	6.247	1513	1526	1561	rVB	492980	1011777	80.11%	7.717%
32	6.398	1561	1573	1605	rVB	51388	122996	9.74%	0.938%
33	6.523	1605	1612	1621	rVB8	2699	5157	0.41%	0.039%
34	6.604	1625	1637	1649	rBV3	8417	20517	1.62%	0.156%
35	6.690	1651	1664	1685	rVB	295861	591411	46.83%	4.511%
36	6.790	1685	1695	1705	rBV2	18658	49622	3.93%	0.378%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050422\
Data File : VU048413.D
Acq On : 04 May 2022 14:44
Operator : SY/MD
Sample : N2639-09
Misc : 5.86g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL19

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	6.935	1733	1740	1750	rBV	18979	42594	3.37%	0.325%
38	7.192	1807	1820	1861	rVV3	77252	244376	19.35%	1.864%
39	7.497	1909	1915	1918	rBV4	534	439	0.03%	0.003%
40	7.510	1918	1919	1924	rVB2	329	233	0.02%	0.002%
41	7.568	1924	1937	1965	rBV	139114	289536	22.93%	2.208%
42	7.693	1971	1976	1982	rBV4	977	1328	0.11%	0.010%
43	7.722	1982	1985	1989	rVB	553	352	0.03%	0.003%
44	7.793	1998	2007	2008	rBV3	2058	2401	0.19%	0.018%
45	7.899	2026	2040	2056	rBV	496744	928562	73.53%	7.082%
46	8.185	2116	2129	2159	rBV4	113123	306468	24.27%	2.337%
47	8.356	2175	2182	2193	rVB8	1250	2408	0.19%	0.018%
48	8.468	2208	2217	2218	rBV3	864	1035	0.08%	0.008%
49	8.552	2231	2243	2254	rBV5	4667	7403	0.59%	0.056%
50	8.677	2260	2282	2310	rBV	375504	919639	72.82%	7.014%
51	8.803	2315	2321	2328	rVB7	2834	4677	0.37%	0.036%
52	8.925	2356	2359	2363	rBV3	616	459	0.04%	0.004%
53	8.983	2374	2377	2379	rBV4	539	366	0.03%	0.003%
54	9.063	2399	2402	2405	rVV2	401	320	0.03%	0.002%
55	9.134	2422	2424	2429	rBV4	430	324	0.03%	0.002%
56	9.156	2429	2431	2439	rVB2	391	358	0.03%	0.003%
57	9.423	2499	2514	2538	rBV	577594	1262906	100.00%	9.632%
58	9.574	2555	2561	2569	rVB7	2852	4242	0.34%	0.032%
59	9.700	2588	2600	2613	rBV2	5922	10783	0.85%	0.082%
60	9.790	2622	2628	2631	rBV2	228	294	0.02%	0.002%
61	10.108	2717	2727	2741	rVV7	4639	9372	0.74%	0.071%
62	10.494	2840	2847	2852	rBV5	1009	1244	0.10%	0.009%
63	10.648	2891	2895	2897	rBV3	521	387	0.03%	0.003%
64	10.661	2897	2899	2904	rVB2	468	310	0.02%	0.002%
65	10.771	2919	2933	2948	rBV	541594	890419	70.51%	6.791%
66	10.896	2964	2972	2983	rBV3	3837	6264	0.50%	0.048%
67	10.941	2983	2986	2992	rVB3	711	645	0.05%	0.005%
68	11.025	3006	3012	3014	rBV3	424	427	0.03%	0.003%
69	11.057	3014	3022	3030	rVV3	24673	36437	2.89%	0.278%
70	11.115	3030	3040	3059	rVB	347279	508830	40.29%	3.881%
71	11.211	3066	3070	3074	rVB4	1203	967	0.08%	0.007%
72	11.282	3088	3092	3094	rVB2	363	258	0.02%	0.002%
73	11.317	3094	3103	3113	rBV7	2537	4671	0.37%	0.036%
74	11.378	3113	3122	3127	rBV7	2679	4230	0.33%	0.032%
75	11.481	3144	3154	3168	rVB7	4185	9925	0.79%	0.076%
76	11.571	3175	3182	3189	rBV6	2451	3978	0.31%	0.030%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050422\
Data File : VU048413.D
Acq On : 04 May 2022 14:44
Operator : SY/MD
Sample : N2639-09
Misc : 5.86g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL19

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	11.603	3190	3192	3198	rVV3	965	724	0.06%	0.006%
78	11.642	3198	3204	3213	rVB7	1644	2656	0.21%	0.020%
79	11.690	3214	3219	3222	rBV4	1208	1170	0.09%	0.009%
80	11.748	3228	3237	3242	rBV6	1558	2519	0.20%	0.019%
81	11.819	3245	3259	3271	rBV	762023	1223057	96.84%	9.328%
82	11.912	3282	3288	3299	rVB2	21347	30335	2.40%	0.231%
83	11.967	3299	3305	3309	rVV6	2415	3528	0.28%	0.027%
84	12.005	3310	3317	3328	rVB3	19472	27383	2.17%	0.209%
85	12.063	3332	3335	3336	rBV2	320	211	0.02%	0.002%
86	12.201	3365	3378	3397	rBV	619525	1014841	80.36%	7.740%
87	12.330	3407	3418	3428	rBV2	68880	99065	7.84%	0.756%
88	12.388	3433	3436	3438	rBV2	636	489	0.04%	0.004%
89	12.523	3475	3478	3481	rBV3	440	358	0.03%	0.003%
90	12.584	3495	3497	3503	rVB2	368	230	0.02%	0.002%
91	12.626	3507	3510	3513	rBV2	305	209	0.02%	0.002%
92	12.774	3547	3556	3566	rBV4	1276	2443	0.19%	0.019%
93	12.899	3590	3595	3600	rBV5	1117	1251	0.10%	0.010%
94	13.053	3641	3643	3647	rVB	482	272	0.02%	0.002%
95	13.221	3692	3695	3698	rBV3	690	528	0.04%	0.004%
96	13.394	3739	3749	3758	rBV3	33506	47682	3.78%	0.364%
97	13.532	3788	3792	3797	rBV4	565	531	0.04%	0.004%
98	13.651	3826	3829	3831	rBV	395	244	0.02%	0.002%
99	15.375	4357	4365	4374	rBV3	14069	18964	1.50%	0.145%
100	15.497	4401	4403	4406	rBV3	996	591	0.05%	0.005%

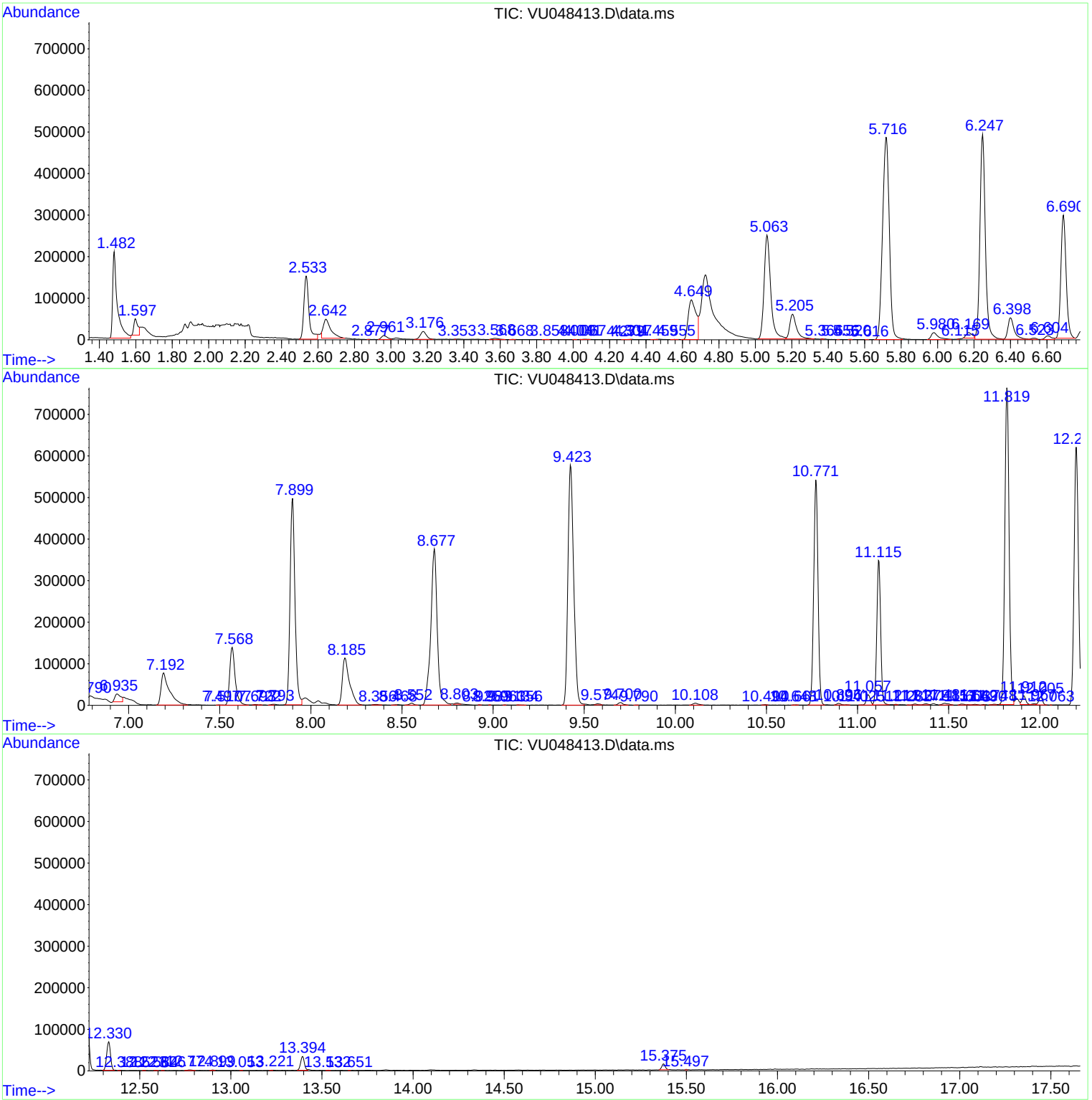
Sum of corrected areas: 13111590

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050422\
Data File : VU048413.D
Acq On : 04 May 2022 14:44
Operator : SY/MD
Sample : N2639-09
Misc : 5.86g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL19

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\VU050422\
Data File : VU048413.D
Acq On : 04 May 2022 14:44
Operator : SY/MD
Sample : N2639-09
Misc : 5.86g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL19

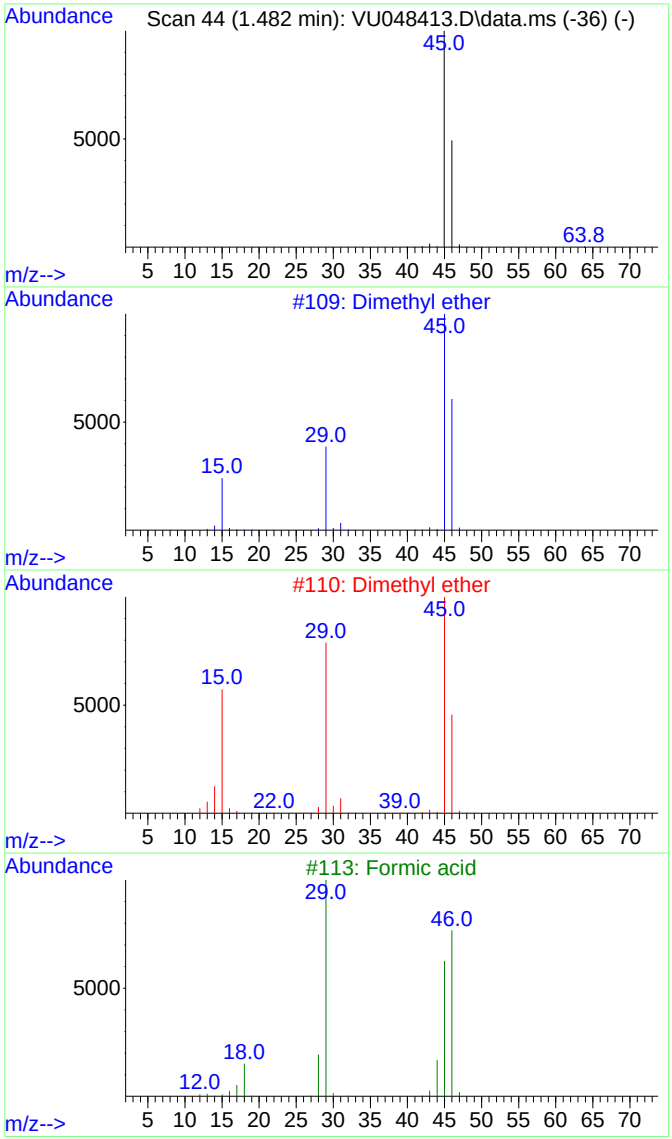
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

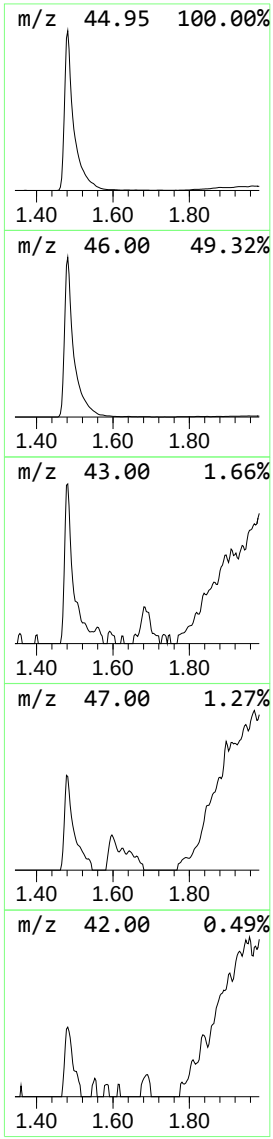
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Dimethyl ether Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.482	18.10 ug/L	366347	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl ether	46	C2H6O	000115-10-6	74
2	Dimethyl ether	46	C2H6O	000115-10-6	74
3	Formic acid	46	CH2O2	000064-18-6	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\VU050422\
Data File : VU048413.D
Acq On : 04 May 2022 14:44
Operator : SY/MD
Sample : N2639-09
Misc : 5.86g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL19

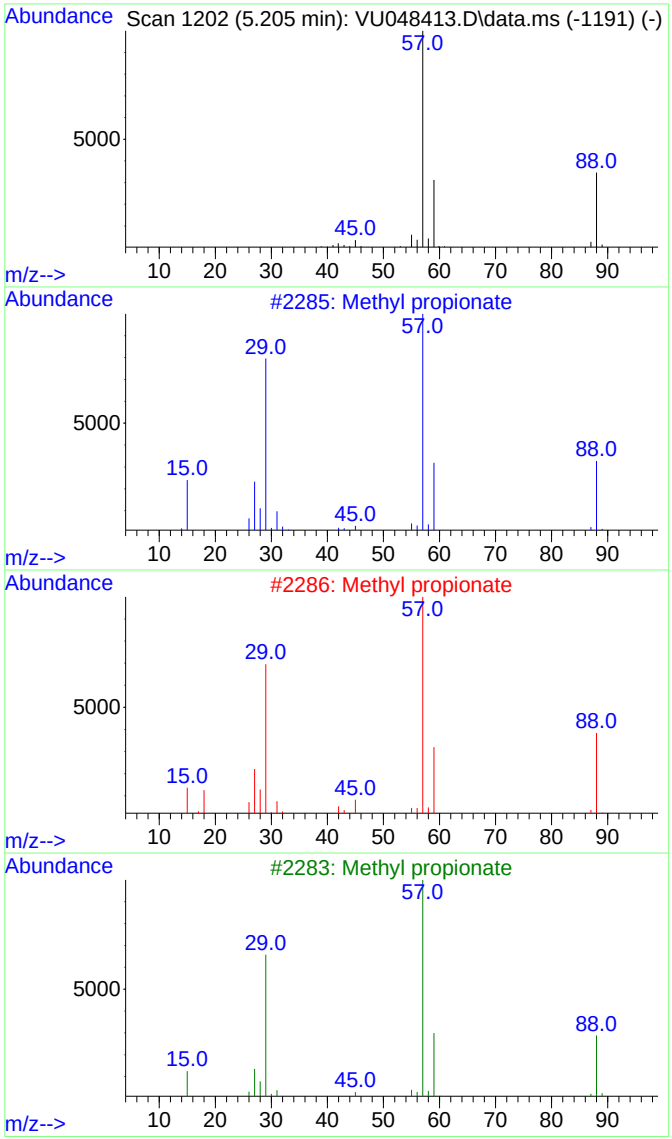
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

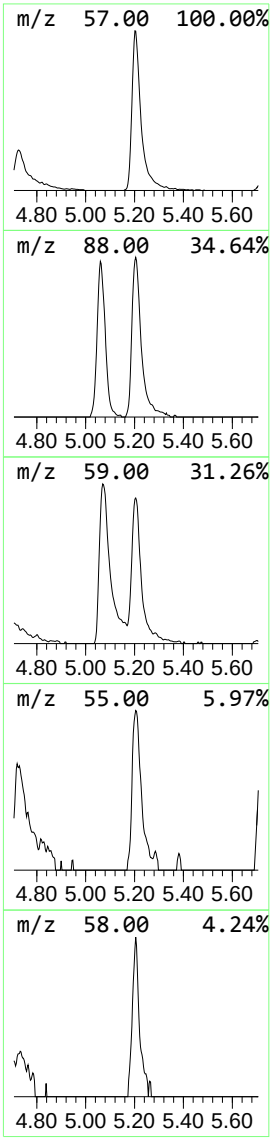
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.205	7.47 ug/L	151059	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	83
4	Methyl propionate	88	C4H8O2	000554-12-1	80
5	Methyl propionate	88	C4H8O2	000554-12-1	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050422\
Data File : VU048413.D
Acq On : 04 May 2022 14:44
Operator : SY/MD
Sample : N2639-09
Misc : 5.86g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL19

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

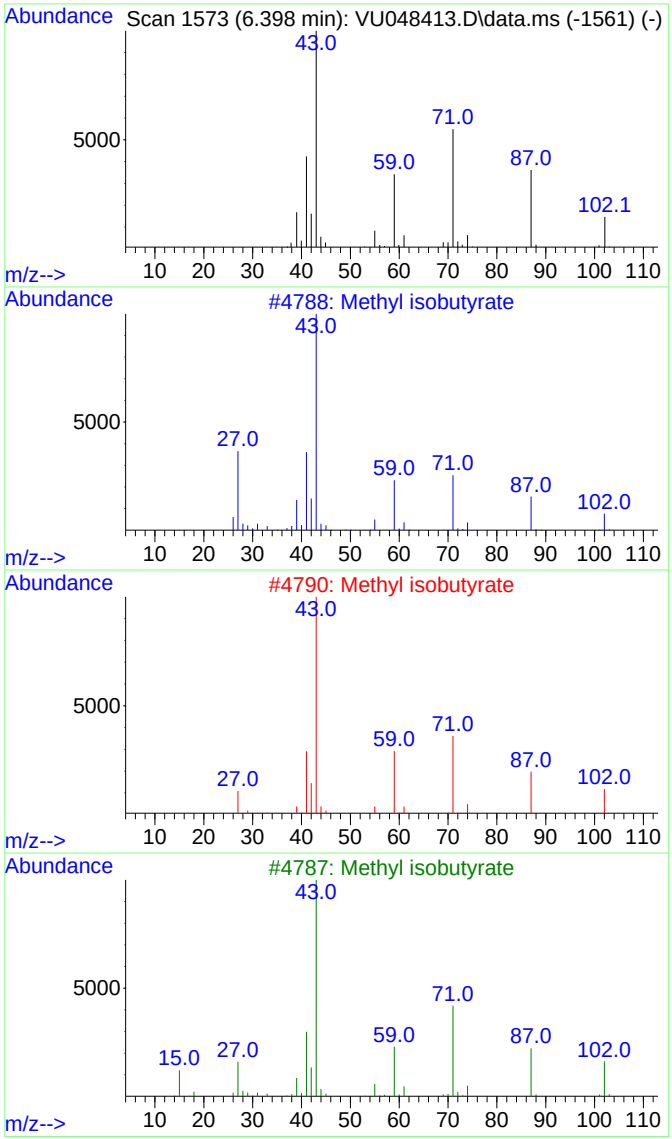
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

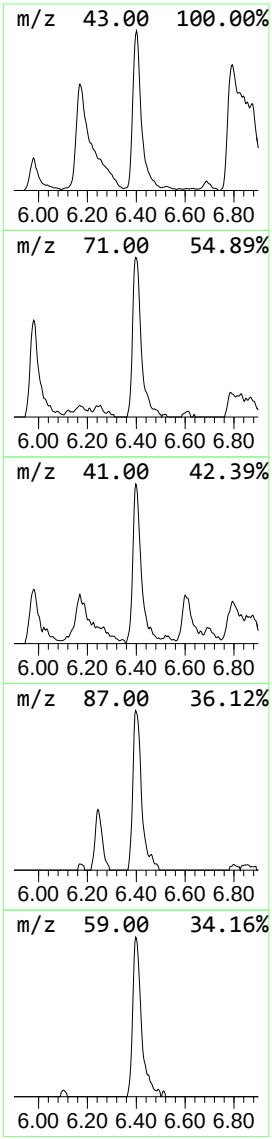
****

Peak Number 3 Methyl isobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.398	6.08 ug/L	122996	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	91
4	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	59
5	Methyl isobutyrate	102	C5H10O2	000547-63-7	58





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050422\
Data File : VU048413.D
Acq On : 04 May 2022 14:44
Operator : SY/MD
Sample : N2639-09
Misc : 5.86g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL19

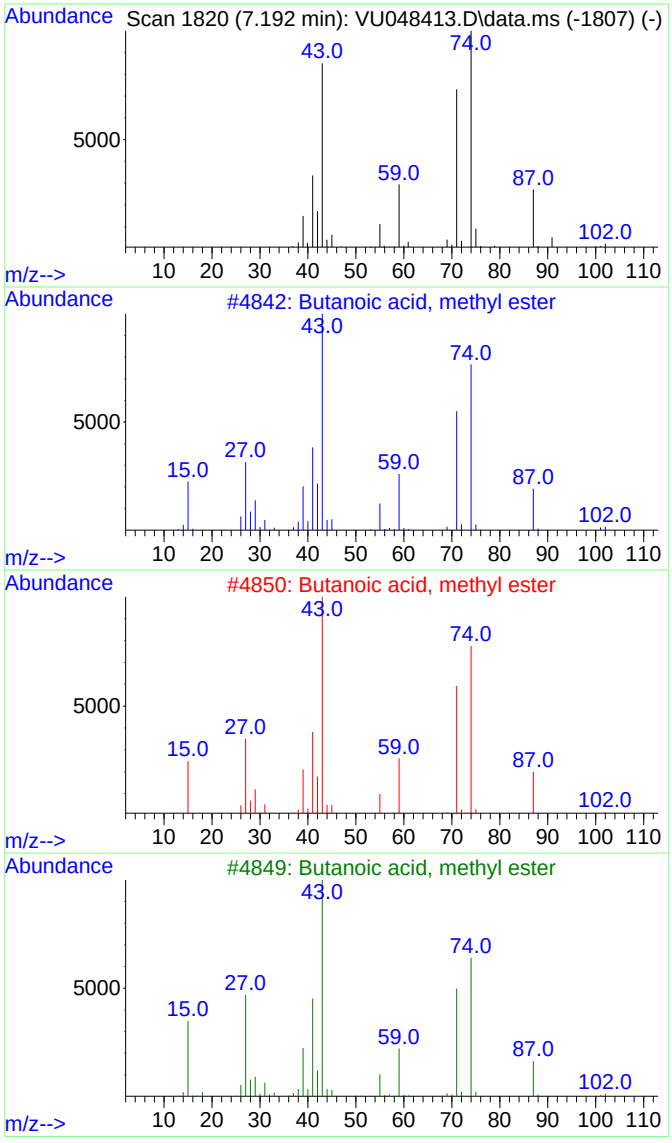
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

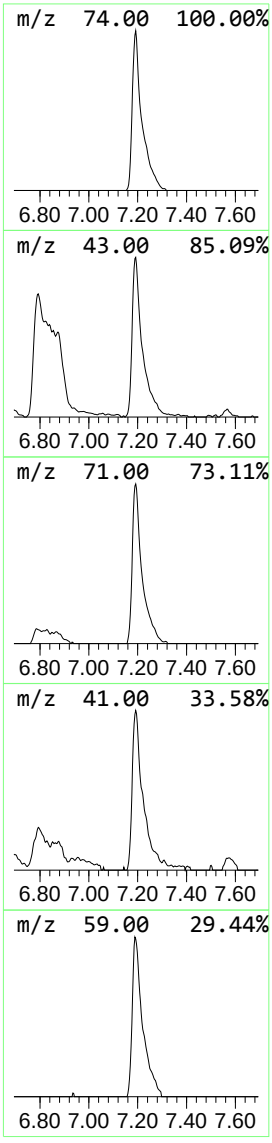
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.192	12.08 ug/L	244376	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	91
2	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	91
3	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	91
4	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	78
5	Hexanoic acid, methyl ester	130	C7H14O2	000106-70-7	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050422\
Data File : VU048413.D
Acq On : 04 May 2022 14:44
Operator : SY/MD
Sample : N2639-09
Misc : 5.86g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL19

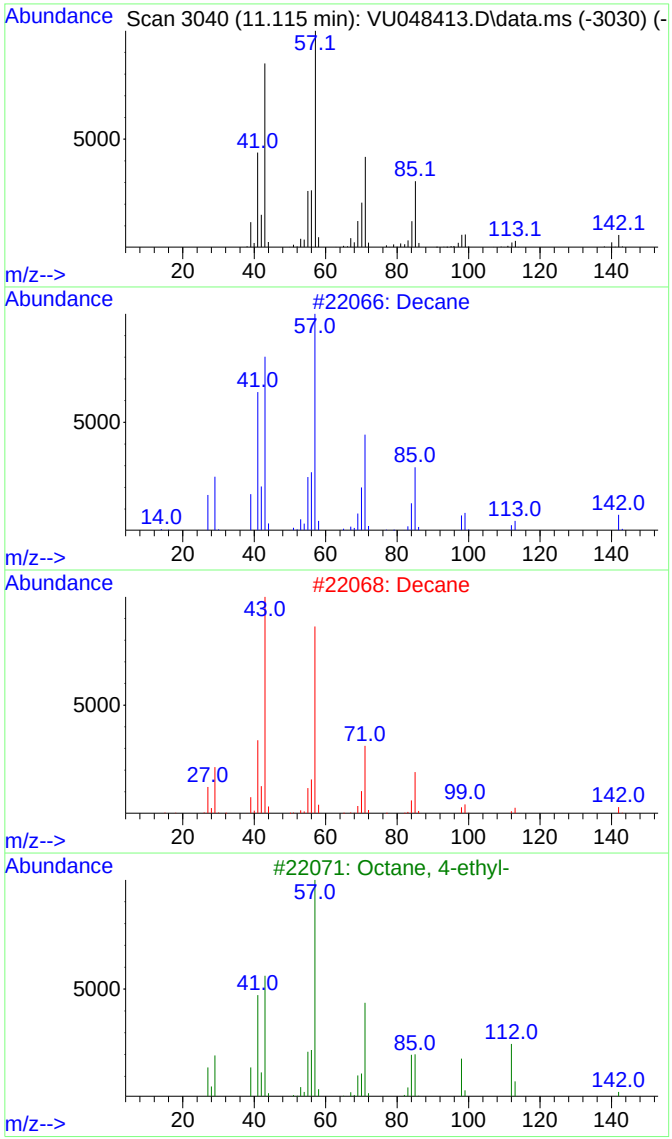
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

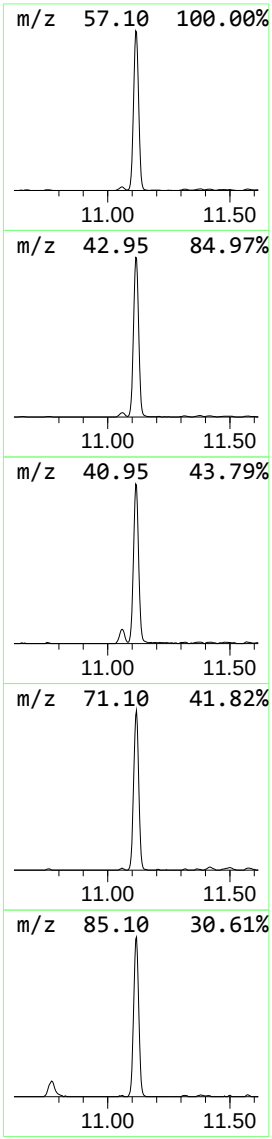
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.115	20.80 ug/L	508830	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane	142	C10H22	000124-18-5	87
2	Decane	142	C10H22	000124-18-5	87
3	Octane, 4-ethyl-	142	C10H22	015869-86-0	72
4	Octane	114	C8H18	000111-65-9	64
5	Decane, 1,1'-oxybis-	298	C20H42O	002456-28-2	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050422\
Data File : VU048413.D
Acq On : 04 May 2022 14:44
Operator : SY/MD
Sample : N2639-09
Misc : 5.86g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL19

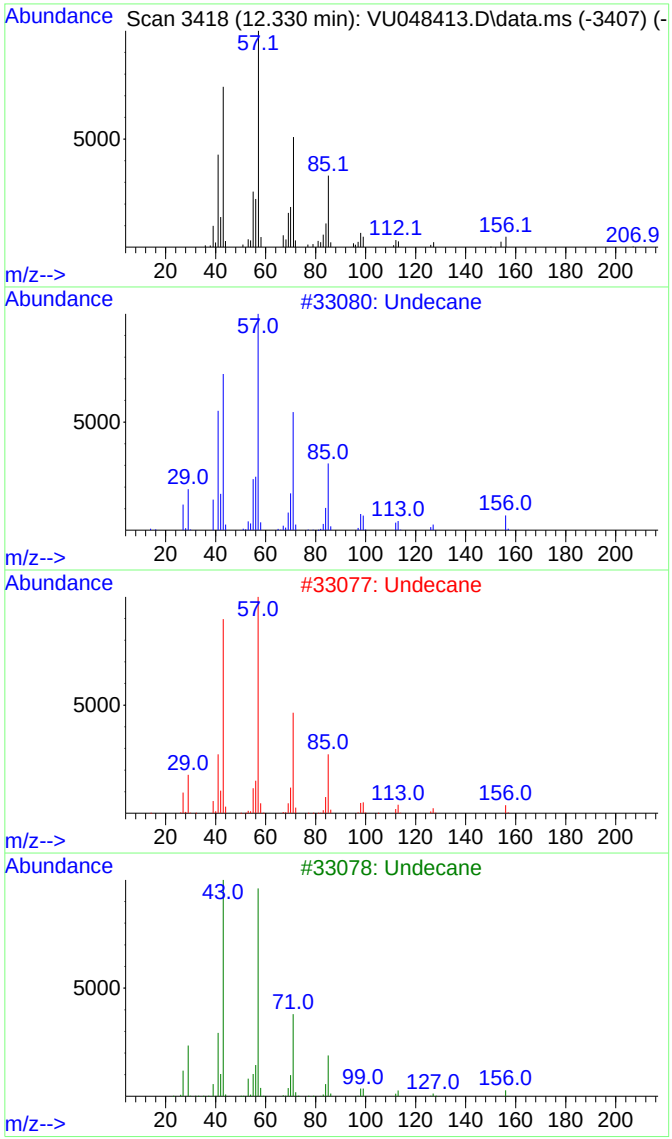
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

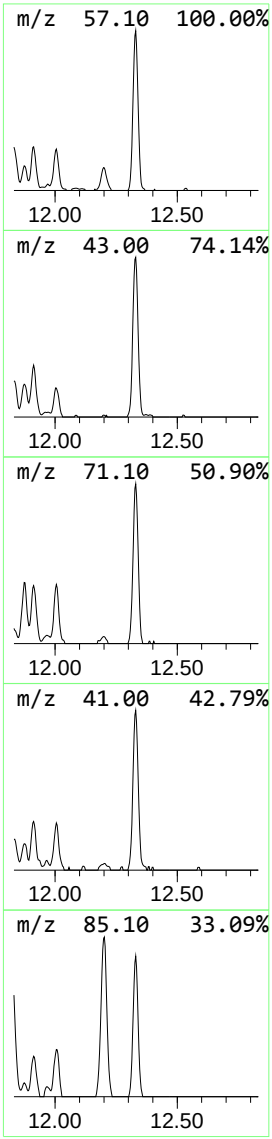
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.330	4.05 ug/L	99065	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	87
2	Undecane	156	C11H24	001120-21-4	83
3	Undecane	156	C11H24	001120-21-4	81
4	Undecane	156	C11H24	001120-21-4	76
5	Undecane	156	C11H24	001120-21-4	70





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050422\
Data File : VU048413.D
Acq On : 04 May 2022 14:44
Operator : SY/MD
Sample : N2639-09
Misc : 5.86g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL19

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	1.482	18.1	ug/L	366347	1	6.247	1011780	50.0
Methyl propionate	5.205	7.5	ug/L	151059	1	6.247	1011780	50.0
Methyl isobutyrate	6.398	6.1	ug/L	122996	1	6.247	1011780	50.0
Butanoic acid, ...	7.192	12.1	ug/L	244376	1	6.247	1011780	50.0
(DEL) Alkane: S...	11.115	20.8	ug/L	508830	3	11.819	1223060	50.0
(DEL) Alkane: S...	12.330	4.0	ug/L	99065	3	11.819	1223060	50.0