LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031723\
Data File : VU053287.D
Acq On : 17 Mar 2023 23:33
Operator : JC/MD
Sample : 01956-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E0234

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\SFAMULM031523WMA.M
Title : VOC Analysis

Signal : TIC: VU053287.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.598	73	80	94	rVB	64173	73943	8.47%	1.600%
2	1.909	169	177	194	rBV	46585	65163	7.46%	1.410%
3	2.562	370	380	393	rBV	87832	140011	16.03%	3.031%
4	3.170	566	569	572	rBV2	439	337	0.04%	0.007%
5	3.353	617	626	632	rBV4	1983	3194	0.37%	0.069%
6	3.485	664	667	670	rBV	197	159	0.02%	0.003%
7	3.549	686	687	688	rBV	121	25	0.00%	0.001%
8	3.642	714	716	719	rVB	216	89	0.01%	0.002%
9	3.697	731	733	734	rBV	287	141	0.02%	0.003%
10	3.771	753	756	759	rBV2	284	175	0.02%	0.004%
11	3.896	791	795	797	rBV	323	273	0.03%	0.006%
12	4.080	845	852	854	rBV3	572	651	0.07%	0.014%
13	4.122	862	865	868	rBV	227	168	0.02%	0.004%
14	4.266	907	910	914	rVB	248	148	0.02%	0.003%
15	4.456	965	969	971	rBV	251	227	0.03%	0.005%
16	4.527	980	991	1002	rVB4	2452	5890	0.67%	0.127%
17	4.613	1005	1018	1029	rBV2	43382	99242	11.36%	2.148%
18	4.819	1076	1082	1085	rBV2	187	239	0.03%	0.005%
19	4.884	1099	1102	1105	rBV2	186	114	0.01%	0.002%
20	4.900	1105	1107	1111	rBV	130	68	0.01%	0.001%
21	4.999	1129	1138	1142	rBV2	1261	1678	0.19%	0.036%
22	5.057	1142	1156	1172	rBV	76713	177260	20.29%	3.837%
23	5.295	1220	1230	1243	rVB7	3182	6863	0.79%	0.149%
24	5.379	1246	1256	1269	rVB5	4910	10940	1.25%	0.237%
25	5.720	1342	1362	1373	rBV2	167719	458005	52.43%	9.913%
26	5.961	1427	1437	1451	rVB4	13716	29130	3.33%	0.631%
27	6.022	1454	1456	1459	rBV4	193	114	0.01%	0.002%
28	6.150	1481	1496	1510	rBV2	4376	10189	1.17%	0.221%
29	6.244	1512	1525	1549	rBV	134676	255316	29.23%	5.526%
30	6.684	1645	1662	1677	rBV	108275	223998	25.64%	4.848%
31	6.883	1714	1724	1733	rBV4	2817	5171	0.59%	0.112%
32	6.919	1733	1735	1736	rBV	232	92	0.01%	0.002%
33	7.154	1788	1808	1830	rBV	64469	144466	16.54%	3.127%
34	7.340	1855	1866	1869	rBV4	2688	4435	0.51%	0.096%
35	7.433	1884	1895	1914	rBV	150605	278116	31.84%	6.020%
36	7.858	2011	2027	2034	rBV	488465	873492	100.00%	18.907%

LSC Area Percent Report

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Data File : VU053287.D
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Operator : JC/MD
Sample : 01956-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E0234

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\SFAMULM031523WMA.M
Title : VOC Analysis

37	8.176	2117	2126	2140	rVB3	48278	85201	9.75%	1.844%
38	8.308	2164	2167	2168	rBV3	662	310	0.04%	0.007%
39	8.359	2177	2183	2186	rBV5	1994	2716	0.31%	0.059%
40	8.485	2211	2222	2237	rBV3	7414	12902	1.48%	0.279%
41	8.572	2237	2249	2256	rBV7	3288	6193	0.71%	0.134%
42	8.629	2256	2267	2297	rBV2	125425	239651	27.44%	5.187%
43	9.006	2382	2384	2386	rBV	250	113	0.01%	0.002%
44	9.131	2418	2423	2429	rBV5	1205	1440	0.16%	0.031%
45	9.186	2429	2440	2456	rVB7	9112	22887	2.62%	0.495%
46	9.266	2456	2465	2476	rVB2	5493	9071	1.04%	0.196%
47	9.327	2476	2484	2495	rBV8	3228	5699	0.65%	0.123%
48	9.414	2498	2511	2517	rBV	192790	341946	39.15%	7.401%
49	9.694	2590	2598	2608	rBV5	2636	3608	0.41%	0.078%
50	9.755	2610	2617	2626	rVB3	1725	2707	0.31%	0.059%
51	9.790	2626	2628	2634	rBV3	337	300	0.03%	0.006%
52	9.835	2641	2642	2644	rBV3	217	99	0.01%	0.002%
53	9.883	2651	2657	2663	rVB4	1146	1452	0.17%	0.031%
54	9.977	2679	2686	2695	rVB3	3519	5525	0.63%	0.120%
55	10.025	2697	2701	2706	rBV4	624	594	0.07%	0.013%
56	10.076	2712	2717	2719	rVB2	300	251	0.03%	0.005%
57	10.096	2720	2723	2725	rBV3	976	760	0.09%	0.016%
58	10.131	2730	2734	2736	rBV	208	98	0.01%	0.002%
59	10.147	2737	2739	2740	rBV	203	57	0.01%	0.001%
60	10.237	2760	2767	2772	rBV3	791	1110	0.13%	0.024%
61	10.356	2794	2804	2814	rBV6	4720	10416	1.19%	0.225%
62	10.478	2831	2842	2851	rBV6	10787	18691	2.14%	0.405%
63	10.536	2853	2860	2872	rVB3	13726	22794	2.61%	0.493%
64	10.642	2881	2893	2906	rBV4	12777	24993	2.86%	0.541%
65	10.751	2917	2927	2951	rVB	152886	258342	29.58%	5.592%
66	10.964	2987	2993	3001	rVB4	4217	5633	0.64%	0.122%
67	11.054	3014	3021	3022	rBV4	1653	1725	0.20%	0.037%
68	11.288	3089	3094	3098	rBV3	1141	1029	0.12%	0.022%
69	11.362	3114	3117	3119	rBV	223	127	0.01%	0.003%
70	11.378	3119	3122	3130	rVB3	414	510	0.06%	0.011%
71	11.433	3131	3139	3144	rVV4	1098	1491	0.17%	0.032%
72	11.465	3148	3149	3155	rVB2	526	298	0.03%	0.006%
73	11.494	3155	3158	3161	rBV2	242	224	0.03%	0.005%
74	11.542	3168	3173	3175	rBV3	802	888	0.10%	0.019%
75	11.568	3179	3181	3183	rVB2	400	145	0.02%	0.003%
76	11.604	3190	3192	3196	rBV3	556	398	0.05%	0.009%

LSC Area Percent Report

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Operator : JC/MD
Sample : 01956-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E0234

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\SFAMULM031523WMA.M
Title : VOC Analysis

77	11.694	3219	3220	3222	rBV3	314	136	0.02%	0.003%
78	11.809	3244	3256	3268	rBV	188001	301147	34.48%	6.518%
79	12.009	3314	3318	3327	rVB6	1396	1627	0.19%	0.035%
80	12.092	3327	3344	3351	rBV6	2358	6019	0.69%	0.130%
81	12.189	3364	3374	3387	rVB	192039	310903	35.59%	6.729%
82	12.349	3419	3424	3427	rBV4	679	807	0.09%	0.017%
83	12.459	3449	3458	3468	rBV7	1688	2875	0.33%	0.062%
84	12.501	3468	3471	3472	rBV3	469	268	0.03%	0.006%
85	12.825	3569	3572	3576	rBV3	436	412	0.05%	0.009%
86	12.944	3607	3609	3610	rBV3	962	357	0.04%	0.008%
87	13.147	3666	3672	3681	rVB5	2491	3738	0.43%	0.081%
88	13.359	3735	3738	3739	rBV	470	219	0.03%	0.005%
89	13.857	3889	3893	3894	rBV	528	390	0.04%	0.008%
90	14.330	4038	4040	4045	rVB4	612	482	0.06%	0.010%
91	14.488	4082	4089	4100	rVB6	17218	27501	3.15%	0.595%
92	14.877	4206	4210	4212	rBV4	677	522	0.06%	0.011%
93	15.137	4287	4291	4296	rBV4	730	726	0.08%	0.016%

Sum of corrected areas: 4620045

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Sample : 01956-01
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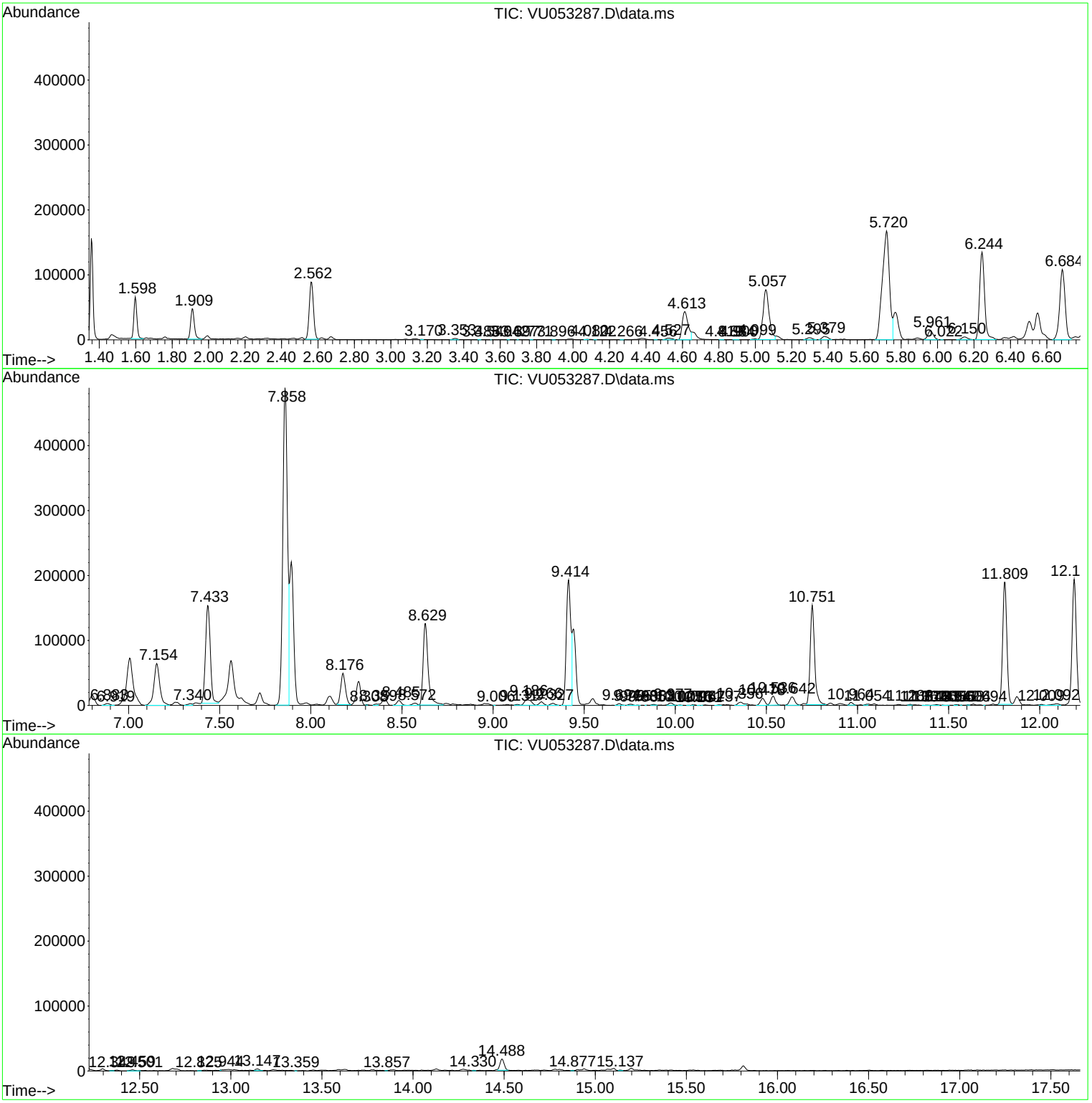
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E0234

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031723\
Data File : VU053287.D
Acq On : 17 Mar 2023 23:33
Operator : JC/MD
Sample : 01956-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E0234

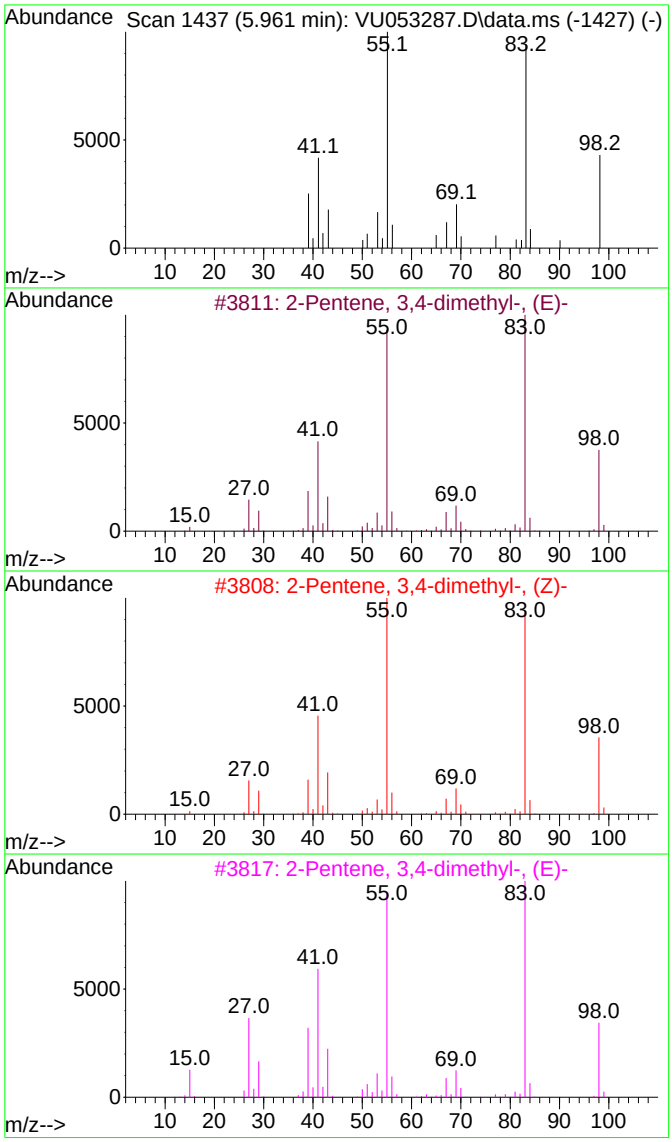
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

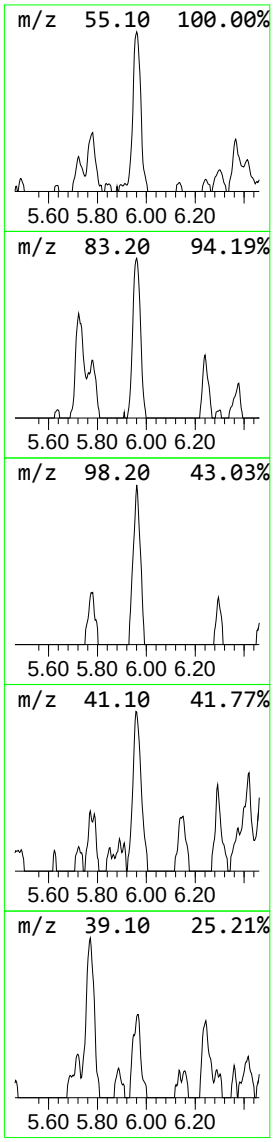
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.961	5.70 ug/L	29130	1,4-Difluorobenzene	6.244

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
2	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	87
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	87
4	2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	87
5	2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	86





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031723\
Data File : VU053287.D
Acq On : 17 Mar 2023 23:33
Operator : JC/MD
Sample : 01956-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E0234

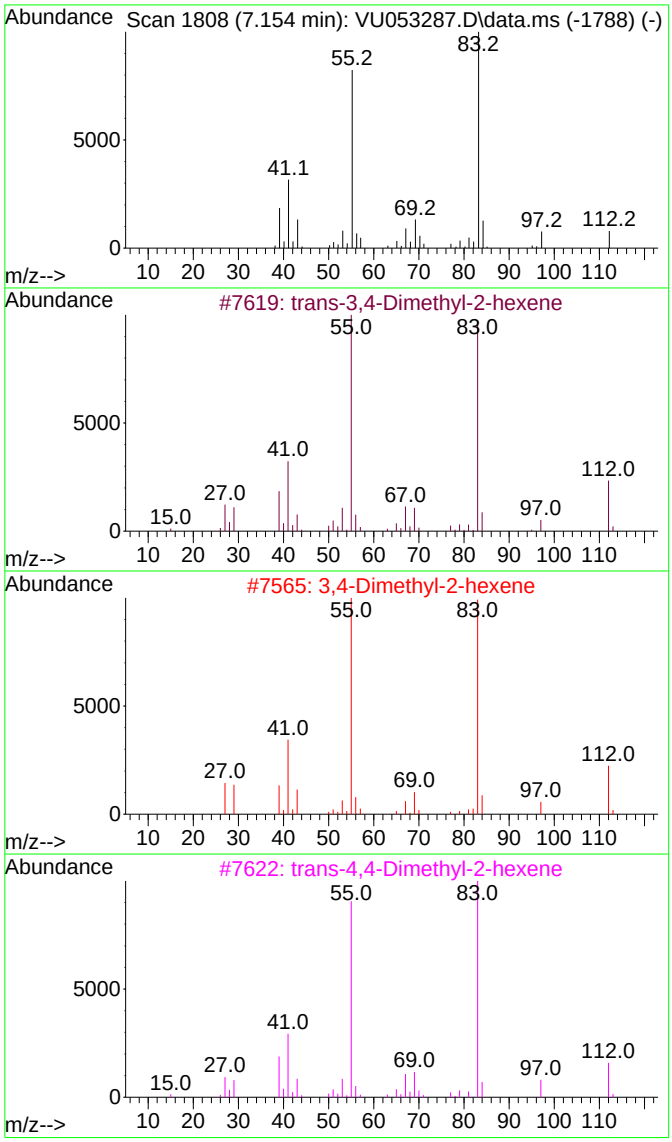
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

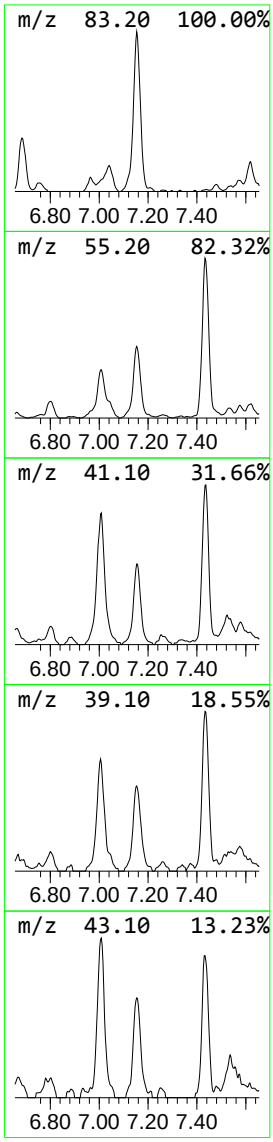
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.154	28.29 ug/L	144466	1,4-Difluorobenzene	6.244

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-3,4-Dimethyl-2-hexene	112	C8H16	019550-82-4	90
2	3,4-Dimethyl-2-hexene	112	C8H16	002213-37-8	90
3	trans-4,4-Dimethyl-2-hexene	112	C8H16	019550-83-5	86
4	2,6-Octadiene, 2,4-dimethyl-	138	C10H18	063843-03-8	72
5	Propanedinitrile, dicyclohexyl-	230	C15H22N2	074764-28-6	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031723\
Data File : VU053287.D
Acq On : 17 Mar 2023 23:33
Operator : JC/MD
Sample : 01956-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E0234

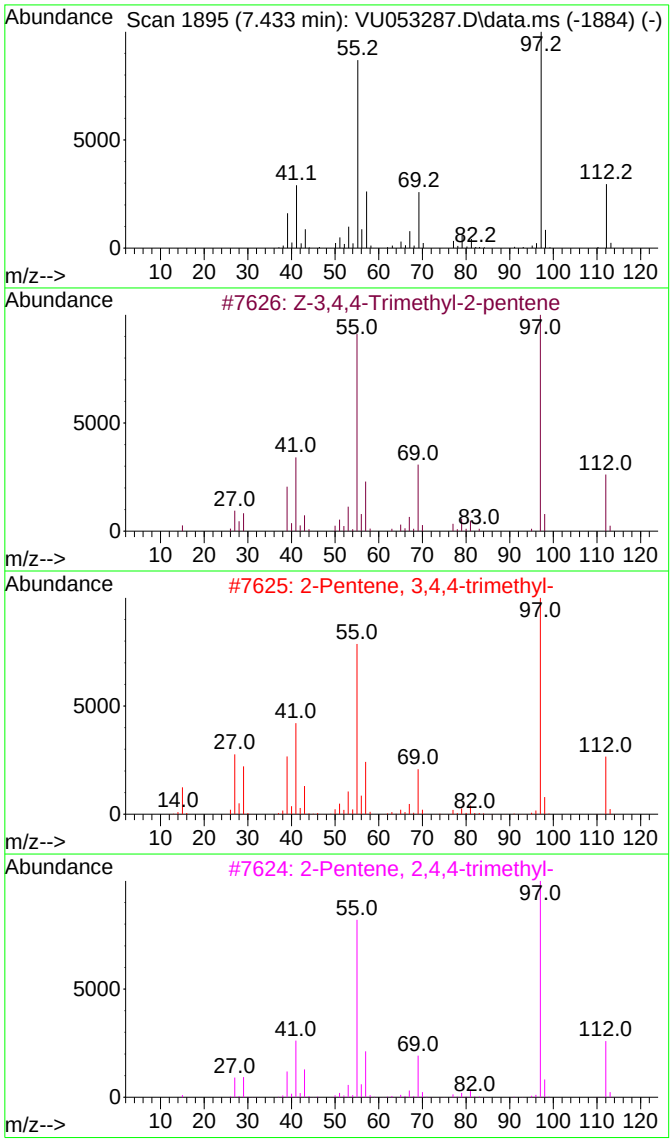
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

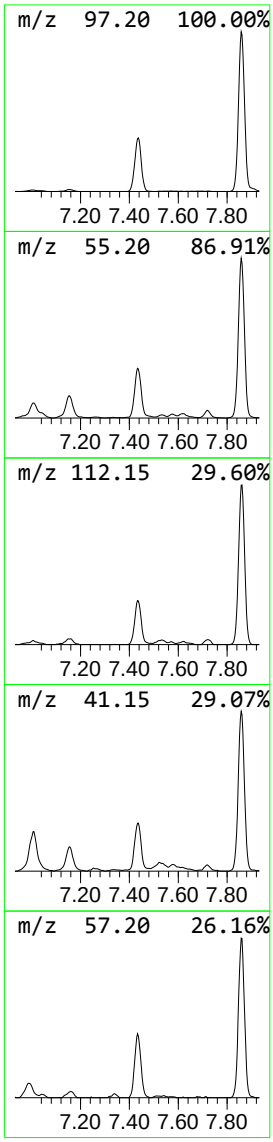
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.433	54.47 ug/L	278116	1,4-Difluorobenzene	6.244

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Z-3,4,4-Trimethyl-2-pentene	112	C8H16	039761-64-3	94
2	2-Pentene, 3,4,4-trimethyl-	112	C8H16	000598-96-9	94
3	2-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-40-4	91
4	2-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-40-4	91
5	2-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-40-4	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031723\
Data File : VU053287.D
Acq On : 17 Mar 2023 23:33
Operator : JC/MD
Sample : 01956-01
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ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E0234

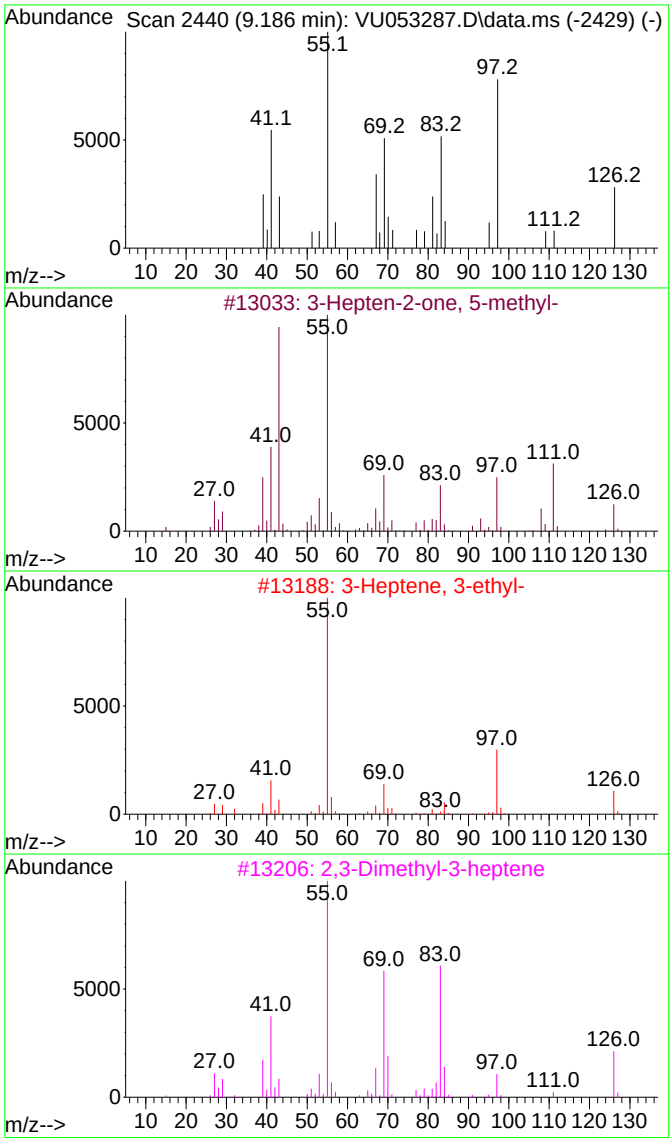
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

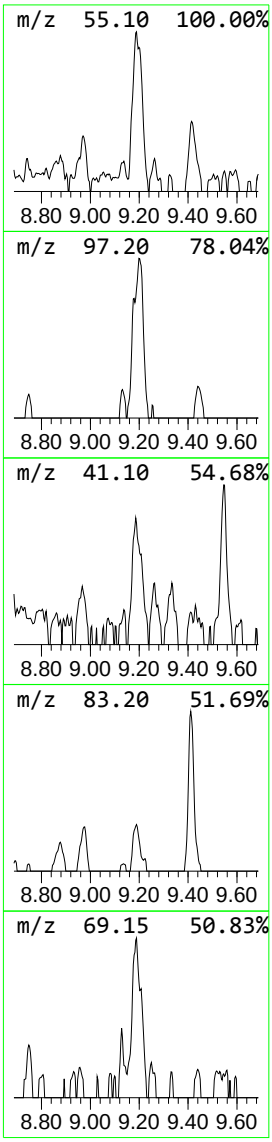
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 3-Hepten-2-one, 5-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.186	3.35 ug/L	22887	Chlorobenzene-d5	9.414

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hepten-2-one, 5-methyl-	126	C8H14O	005090-16-4	59
2	3-Heptene, 3-ethyl-	126	C9H18	074764-46-8	50
3	2,3-Dimethyl-3-heptene	126	C9H18	1000113-49-3	46
4	Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	43
5	Cyclopentane, 2-isopropyl-1,3-di...	140	C10H20	032281-85-9	42





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031723\
Data File : VU053287.D
Acq On : 17 Mar 2023 23:33
Operator : JC/MD
Sample : 01956-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E0234

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

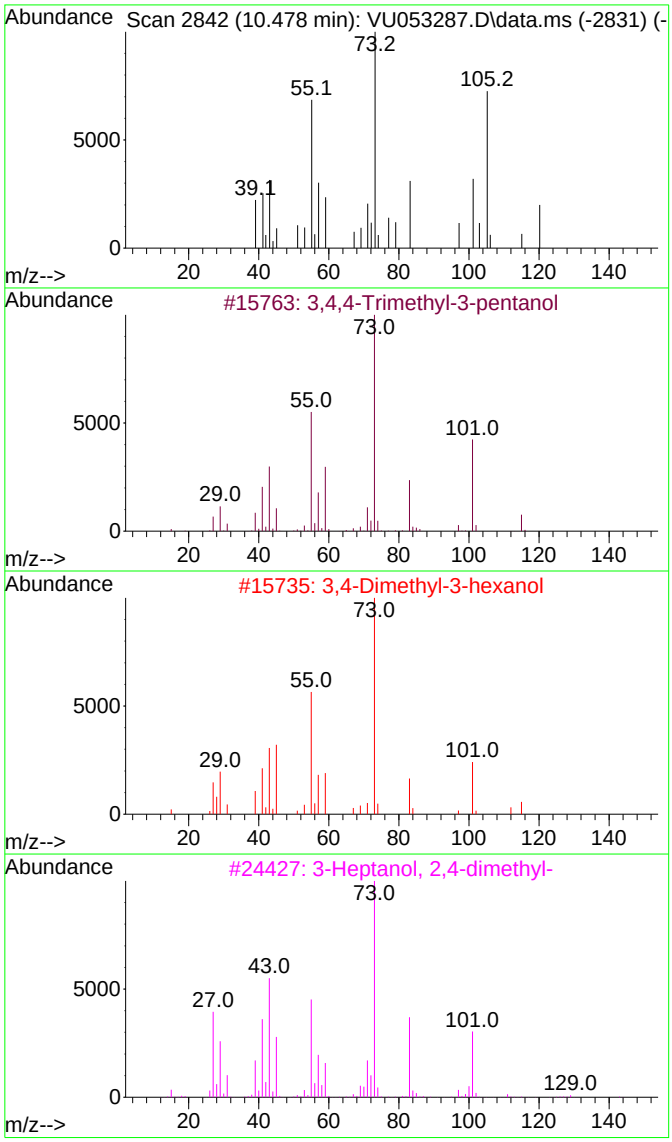
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

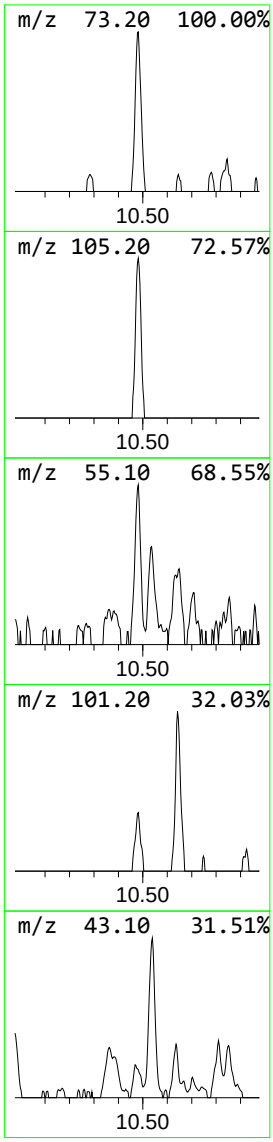
****

Peak Number 5 unknown-01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.478	2.73 ug/L	18691	Chlorobenzene-d5	9.414

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4,4-Trimethyl-3-pentanol	130	C8H18O	007294-05-5	32
2	3,4-Dimethyl-3-hexanol	130	C8H18O	019550-08-4	32
3	3-Heptanol, 2,4-dimethyl-	144	C9H20O	019549-72-5	28
4	3,4-Dimethyl-3-hexanol	130	C8H18O	019550-08-4	25
5	3-Heptanol, 2,4-dimethyl-	144	C9H20O	019549-72-5	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031723\
Data File : VU053287.D
Acq On : 17 Mar 2023 23:33
Operator : JC/MD
Sample : 01956-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E0234

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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

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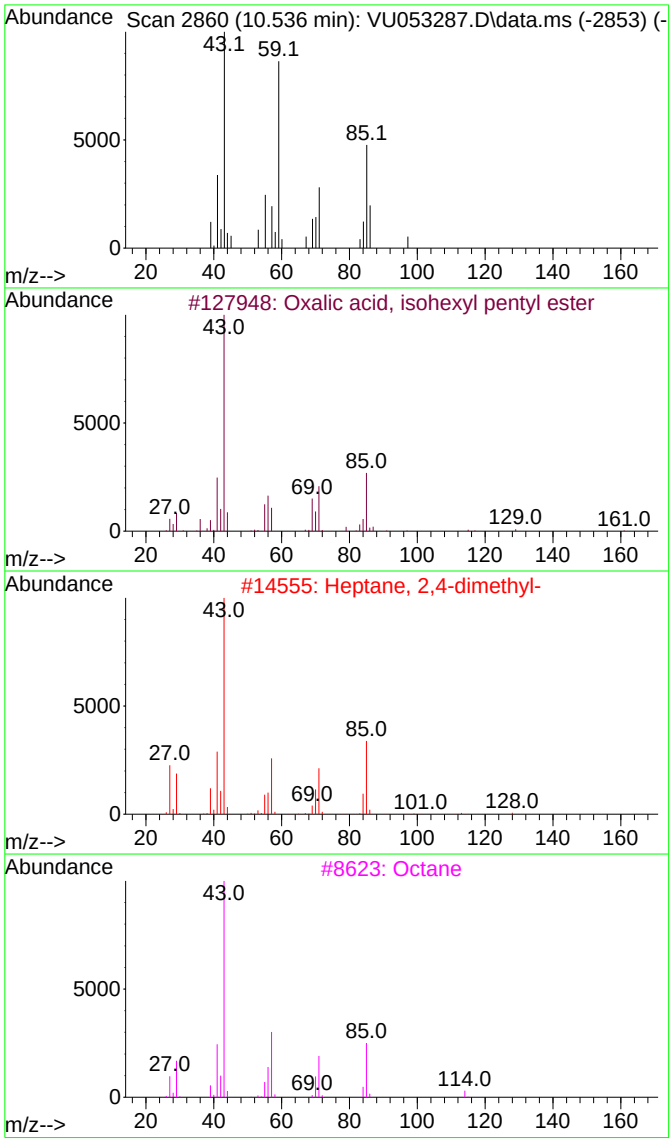
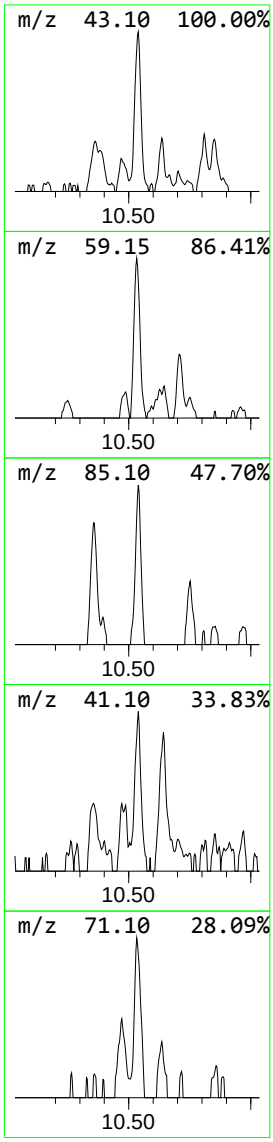
Peak Number 6 unknown-02 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.536	3.33 ug/L	22794	Chlorobenzene-d5	9.414

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isohexyl pentyl ester	244	C13H24O4	1000309-32-8	32
2	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	25
3	Octane	114	C8H18	000111-65-9	25
4	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	25
5	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031723\
Data File : VU053287.D
Acq On : 17 Mar 2023 23:33
Operator : JC/MD
Sample : 01956-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E0234

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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

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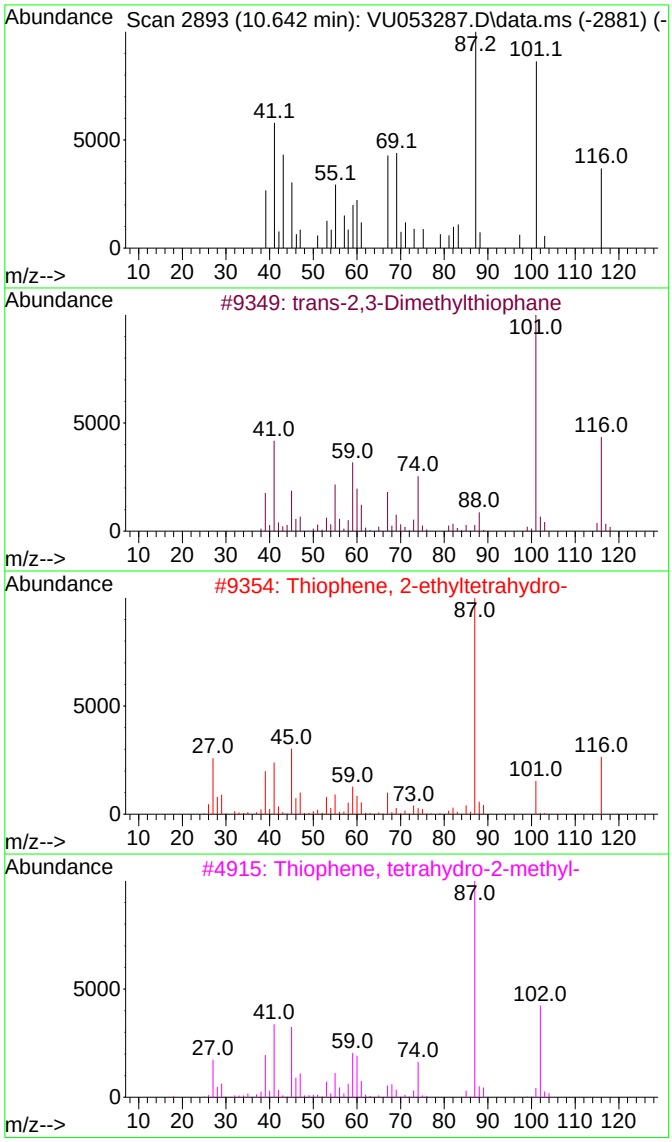
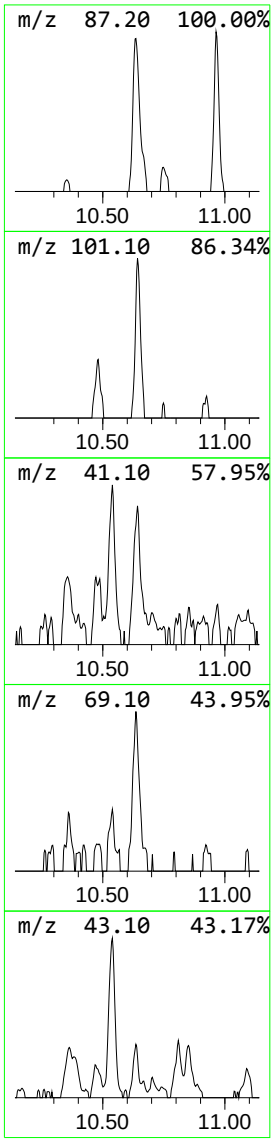
Peak Number 7 unknown-03 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.642	4.15 ug/L	24993	1,4-Dichlorobenzene-d4	11.809

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	46
2	Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	43
3	Thiophene, tetrahydro-2-methyl-	102	C5H10S	001795-09-1	38
4	Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	38
5	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031723\
Data File : VU053287.D
Acq On : 17 Mar 2023 23:33
Operator : JC/MD
Sample : 01956-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E0234

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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

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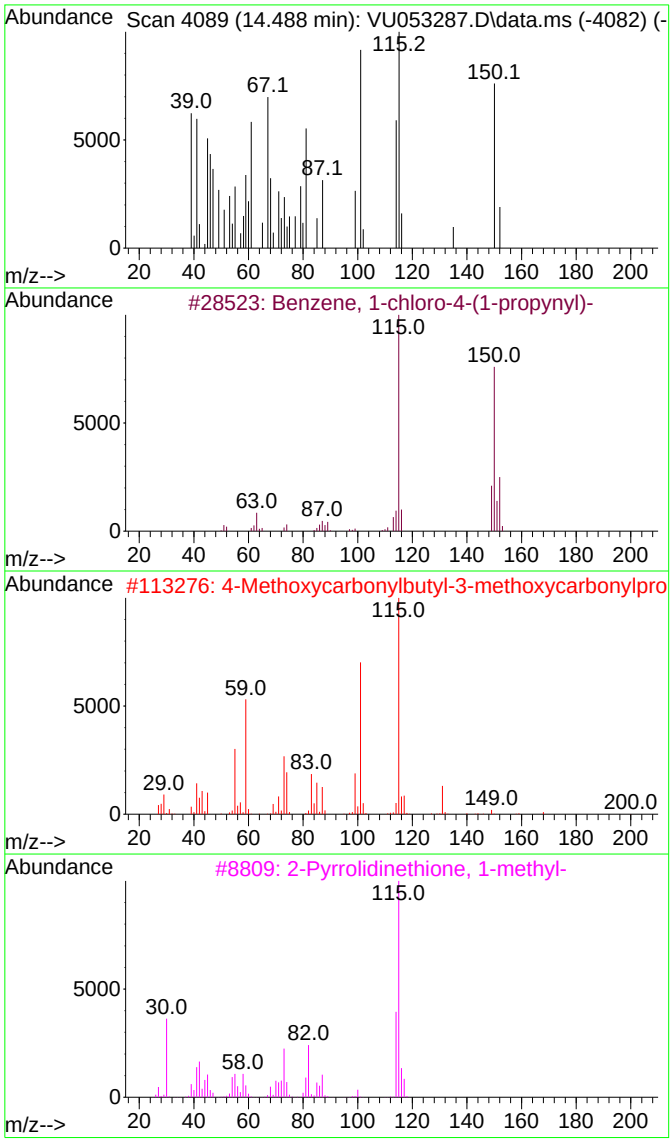
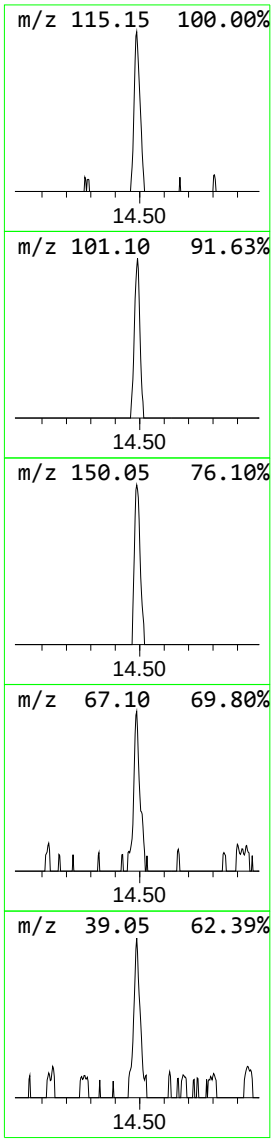
Peak Number 8 unknown-04 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.488	4.57 ug/L	27501	1,4-Dichlorobenzene-d4	11.809

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-chloro-4-(1-propynyl)-	150	C9H7Cl	002809-65-6	38
2	4-Methoxycarbonylbutyl-3-methoxy...	232	C11H20O5	017361-53-4	12
3	2-Pyrrolidinethione, 1-methyl-	115	C5H9NS	010441-57-3	11
4	2-Piperidinethione	115	C5H9NS	013070-01-4	10
5	1H-Pyrazole, 3-methyl-5-(trifluo...	150	C5H5F3N2	010010-93-2	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031723\
Data File : VU053287.D
Acq On : 17 Mar 2023 23:33
Operator : JC/MD
Sample : 01956-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E0234

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.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
(DEL) Alkane: S...	5.961	5.7	ug/L	29130	1	6.244	255316	50.0
(DEL) Alkane: S...	7.154	28.3	ug/L	144466	1	6.244	255316	50.0
(DEL) Alkane: S...	7.433	54.5	ug/L	278116	1	6.244	255316	50.0
3-Hepten-2-one,...	9.186	3.4	ug/L	22887	2	9.414	341946	50.0
unknown-01	10.478	2.7	ug/L	18691	2	9.414	341946	50.0
unknown-02	10.536	3.3	ug/L	22794	2	9.414	341946	50.0
unknown-03	10.642	4.2	ug/L	24993	3	11.809	301147	50.0
unknown-04	14.488	4.6	ug/L	27501	3	11.809	301147	50.0