LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121423\
Data File : VV033351.D
Acq On : 14 Dec 2023 21:46
Operator : SY/MD
Sample : 05807-06 100X
Misc : 2.55g/5.0mL/100uL/5.00mL/MSVOA_V/MEOH
ALS Vial : 30 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AX8

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_V\Method\SFAMVLM120123WMA.M
Title : VOC Analysis

Signal : TIC: VV033351.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.214	361	365	368	rBB2	360	238	0.03%	0.007%
2	2.240	369	373	375	rBV2	413	352	0.05%	0.010%
3	2.314	392	396	398	rBB	246	161	0.02%	0.004%
4	2.330	399	401	403	rBV	261	145	0.02%	0.004%
5	2.452	430	439	445	rBB3	1263	1909	0.27%	0.053%
6	2.487	446	450	453	rBB	122	105	0.01%	0.003%
7	2.516	456	459	462	rBV	243	197	0.03%	0.005%
8	2.680	508	510	513	rBB	162	110	0.02%	0.003%
9	2.725	521	524	526	rBB	186	119	0.02%	0.003%
10	2.751	529	532	535	rBB	163	102	0.01%	0.003%
11	2.835	556	558	561	rBV	138	116	0.02%	0.003%
12	2.970	597	600	602	rBB	253	141	0.02%	0.004%
13	3.748	840	842	845	rBB	167	108	0.02%	0.003%
14	3.786	845	854	884	rBV	36107	101272	14.16%	2.798%
15	4.506	1075	1078	1081	rBV	219	203	0.03%	0.006%
16	4.568	1093	1097	1098	rBV	271	167	0.02%	0.005%
17	4.596	1102	1106	1107	rBV	164	129	0.02%	0.004%
18	4.632	1115	1117	1119	rBB	238	94	0.01%	0.003%
19	4.770	1158	1160	1162	rBB	242	93	0.01%	0.003%
20	4.854	1184	1186	1188	rBV	176	120	0.02%	0.003%
21	4.957	1201	1218	1245	rBV4	267299	714949	100.00%	19.751%
22	5.494	1382	1385	1386	rBV	249	142	0.02%	0.004%
23	6.172	1595	1596	1599	rBV	491	305	0.04%	0.008%
24	6.204	1604	1606	1608	rBB	266	120	0.02%	0.003%
25	6.323	1639	1643	1645	rBB	244	180	0.03%	0.005%
26	6.416	1666	1672	1674	rBB	169	181	0.03%	0.005%
27	6.532	1706	1708	1711	rBB	226	111	0.02%	0.003%
28	6.606	1727	1731	1734	rBV	181	199	0.03%	0.005%
29	6.696	1754	1759	1762	rBB	170	159	0.02%	0.004%
30	6.751	1773	1776	1778	rBB	238	110	0.02%	0.003%
31	6.912	1816	1826	1850	rBV2	85426	160927	22.51%	4.446%
32	7.092	1881	1882	1886	rVB	376	186	0.03%	0.005%
33	7.111	1886	1888	1890	rBV	368	165	0.02%	0.005%
34	7.137	1894	1896	1897	rBV	349	132	0.02%	0.004%
35	7.879	2118	2127	2138	rBB4	1006	1731	0.24%	0.048%
36	7.934	2142	2144	2146	rBV	135	93	0.01%	0.003%

LSC Area Percent Report

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Operator : SY/MD
Sample : 05807-06 100X
Misc : 2.55g/5.0mL/100uL/5.00mL/MSVOA_V/MEOH
ALS Vial : 30 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0AX8

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_V\Method\SFAMVLM120123WMA.M
Title : VOC Analysis

37	8.024	2163	2172	2210	rBV	132195	253411	35.44%	7.001%
38	8.355	2268	2275	2276	rBV3	1068	939	0.13%	0.026%
39	8.416	2290	2294	2296	rBV	171	132	0.02%	0.004%
40	8.567	2339	2341	2343	rBB	221	102	0.01%	0.003%
41	8.590	2344	2348	2349	rBV	328	152	0.02%	0.004%
42	8.625	2357	2359	2362	rBV	132	117	0.02%	0.003%
43	8.786	2397	2409	2444	rBV	366908	629101	87.99%	17.380%
44	9.082	2498	2501	2504	rBV3	409	275	0.04%	0.008%
45	9.165	2524	2527	2529	rBV2	250	144	0.02%	0.004%
46	9.246	2550	2552	2554	rBB	288	146	0.02%	0.004%
47	9.297	2565	2568	2571	rBB	180	135	0.02%	0.004%
48	9.349	2582	2584	2587	rBV	151	126	0.02%	0.003%
49	9.625	2666	2670	2672	rBB	157	106	0.01%	0.003%
50	9.722	2698	2700	2704	rBB	151	125	0.02%	0.003%
51	9.860	2740	2743	2746	rBB	136	120	0.02%	0.003%
52	9.879	2746	2749	2751	rBB	264	187	0.03%	0.005%
53	9.927	2762	2764	2766	rBV	152	101	0.01%	0.003%
54	10.153	2823	2834	2856	rBV	236759	366478	51.26%	10.124%
55	10.275	2868	2872	2875	rBV2	296	257	0.04%	0.007%
56	10.445	2922	2925	2926	rBB	213	102	0.01%	0.003%
57	10.493	2936	2940	2942	rBB	208	133	0.02%	0.004%
58	10.577	2964	2966	2968	rBV	220	129	0.02%	0.004%
59	10.632	2980	2983	2988	rBB	151	176	0.02%	0.005%
60	10.680	2996	2998	3001	rBV	239	140	0.02%	0.004%
61	10.760	3019	3023	3028	rBV	149	226	0.03%	0.006%
62	10.953	3081	3083	3086	rBB	136	95	0.01%	0.003%
63	11.030	3104	3107	3109	rBB	181	116	0.02%	0.003%
64	11.101	3127	3129	3133	rBB	219	107	0.01%	0.003%
65	11.130	3134	3138	3144	rBB2	343	334	0.05%	0.009%
66	11.185	3144	3155	3184	rBV	430599	679902	95.10%	18.783%
67	11.400	3220	3222	3224	rBB	248	114	0.02%	0.003%
68	11.413	3225	3226	3228	rBV	246	101	0.01%	0.003%
69	11.561	3260	3272	3295	rBV	445607	690907	96.64%	19.087%
70	11.831	3353	3356	3358	rBV	171	128	0.02%	0.004%
71	11.940	3387	3390	3393	rBV2	289	260	0.04%	0.007%
72	11.979	3399	3402	3404	rBB	215	109	0.02%	0.003%
73	12.024	3413	3416	3419	rBV	171	157	0.02%	0.004%
74	12.082	3432	3434	3437	rBB	267	146	0.02%	0.004%
75	12.133	3447	3450	3454	rBB2	316	292	0.04%	0.008%
76	12.355	3516	3519	3522	rBB	168	136	0.02%	0.004%

LSC Area Percent Report

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Operator : SY/MD
Sample : 05807-06 100X
Misc : 2.55g/5.0mL/100uL/5.00mL/MSVOA_V/MEOH
ALS Vial : 30 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0AX8

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_V\Method\SFAMVLM120123WMA.M
Title : VOC Analysis

77	12.445	3546	3547	3551	rBB	143	96	0.01%	0.003%
78	12.471	3552	3555	3557	rBB	137	94	0.01%	0.003%
79	12.545	3572	3578	3579	rBB	266	199	0.03%	0.005%
80	12.590	3585	3592	3599	rBB4	517	662	0.09%	0.018%
81	12.638	3604	3607	3609	rBB	203	104	0.01%	0.003%
82	12.680	3616	3620	3623	rBB2	381	214	0.03%	0.006%
83	12.741	3637	3639	3640	rBV	255	121	0.02%	0.003%
84	12.779	3647	3651	3654	rBB	378	277	0.04%	0.008%
85	12.828	3663	3666	3667	rBV	260	153	0.02%	0.004%
86	12.869	3677	3679	3681	rBV2	349	206	0.03%	0.006%
87	12.937	3695	3700	3702	rBB	239	178	0.02%	0.005%
88	13.095	3746	3749	3753	rBV	323	211	0.03%	0.006%
89	13.201	3779	3782	3783	rBV	608	312	0.04%	0.009%
90	13.287	3807	3809	3812	rBB2	321	189	0.03%	0.005%
91	13.316	3813	3818	3819	rBV2	388	243	0.03%	0.007%
92	13.345	3825	3827	3829	rBB	247	114	0.02%	0.003%
93	13.365	3832	3833	3836	rBB	237	102	0.01%	0.003%
94	13.390	3839	3841	3844	rBB2	374	230	0.03%	0.006%
95	13.455	3851	3861	3867	rBV5	2014	3176	0.44%	0.088%
96	13.590	3901	3903	3905	rBV	358	191	0.03%	0.005%
97	13.966	4015	4020	4021	rBV3	635	617	0.09%	0.017%
98	14.069	4050	4052	4054	rBV	441	278	0.04%	0.008%
99	14.140	4071	4074	4076	rBB	251	144	0.02%	0.004%
100	14.156	4077	4079	4081	rBV	228	109	0.02%	0.003%

Sum of corrected areas: 3619755

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121423\
Data File : VV033351.D
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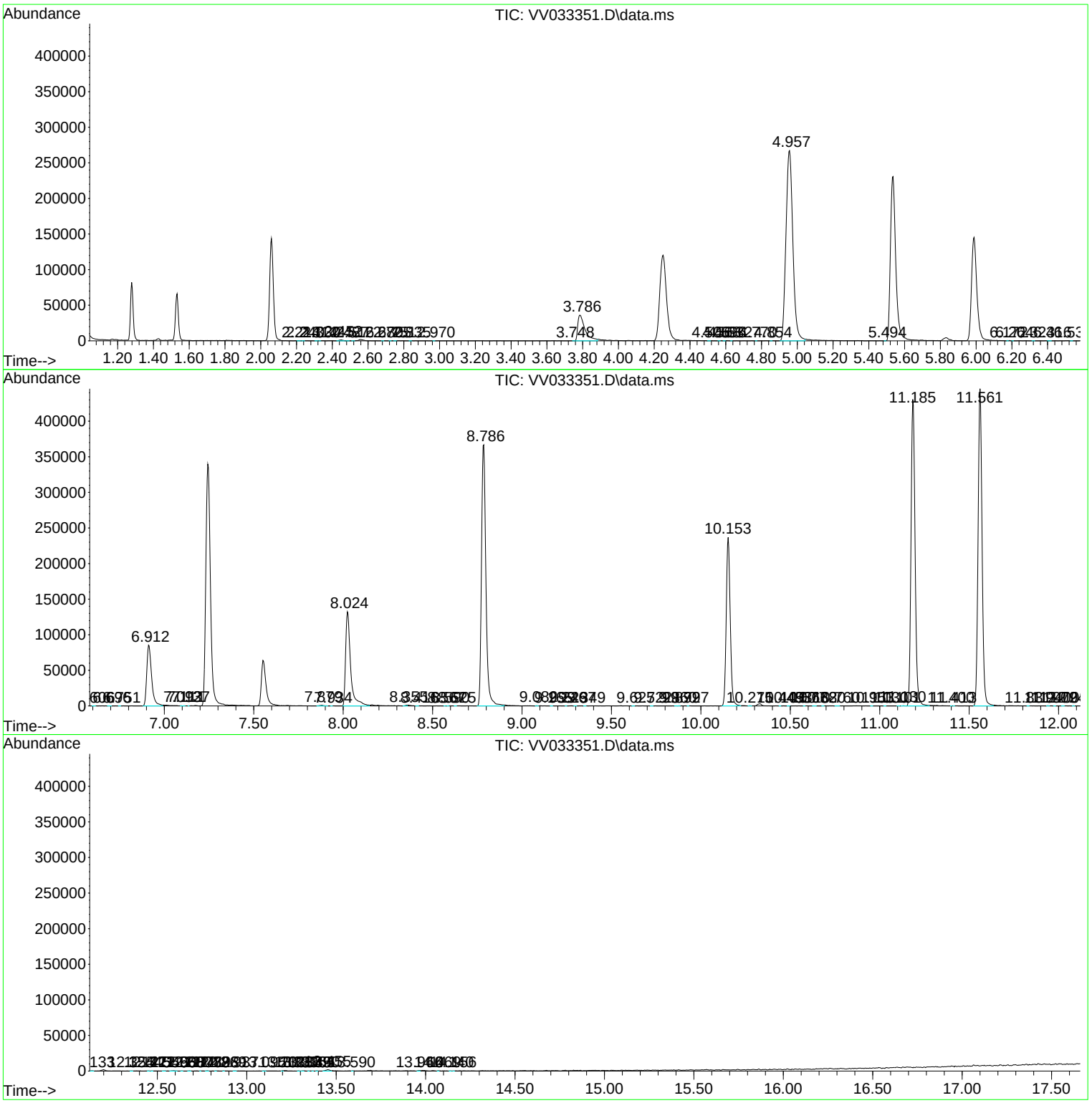
Operator : SY/MD
Sample : 05807-06 100X
Misc : 2.55g/5.0mL/100uL/5.00mL/MSVOA_V/MEOH
ALS Vial : 30 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AX8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121423\
Data File : VV033351.D
Acq On : 14 Dec 2023 21:46
Operator : SY/MD
Sample : 05807-06 100X
Misc : 2.55g/5.0mL/100uL/5.00mL/MSVOA_V/MEOH
ALS Vial : 30 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AX8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

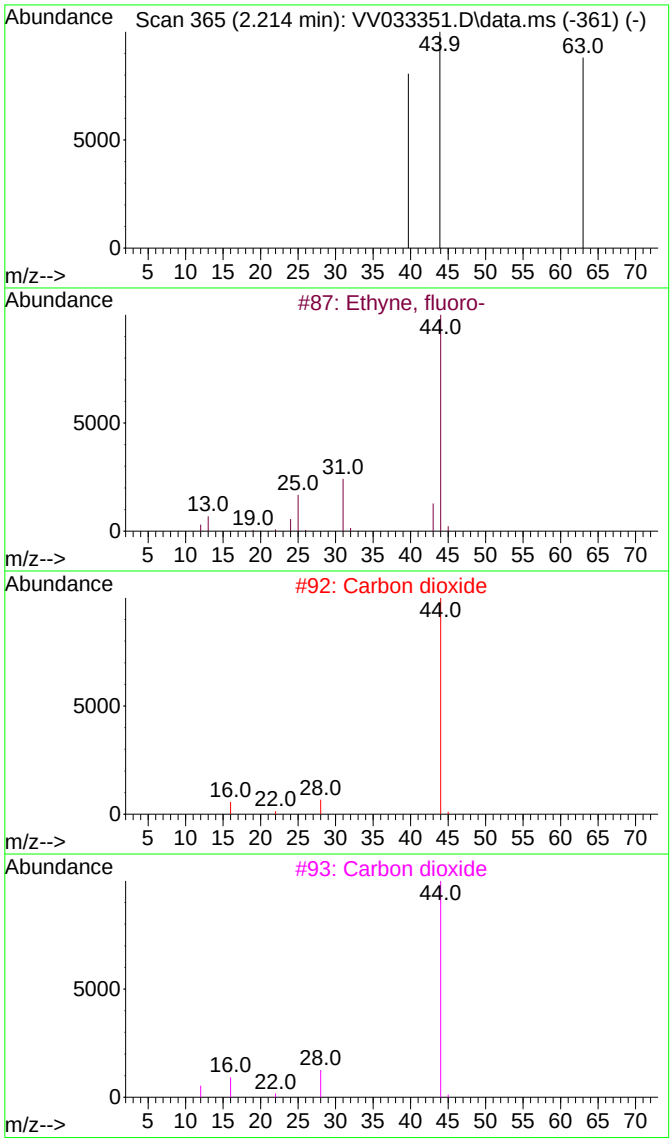
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

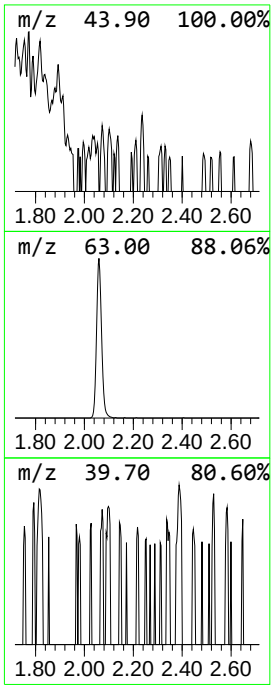
****

Peak Number 1 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.214	83.80 ug/L	238	1,4-Difluorobenzene	5.535

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyne, fluoro-	44	C2HF	002713-09-9	2
2	Carbon dioxide	44	CO2	000124-38-9	2
3	Carbon dioxide	44	CO2	000124-38-9	2
4	Ethyne, fluoro-	44	C2HF	002713-09-9	2
5	Acetaldehyde	44	C2H4O	000075-07-0	2





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121423\
Data File : VV033351.D
Acq On : 14 Dec 2023 21:46
Operator : SY/MD
Sample : 05807-06 100X
Misc : 2.55g/5.0mL/100uL/5.00mL/MSVOA_V/MEOH
ALS Vial : 30 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AX8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

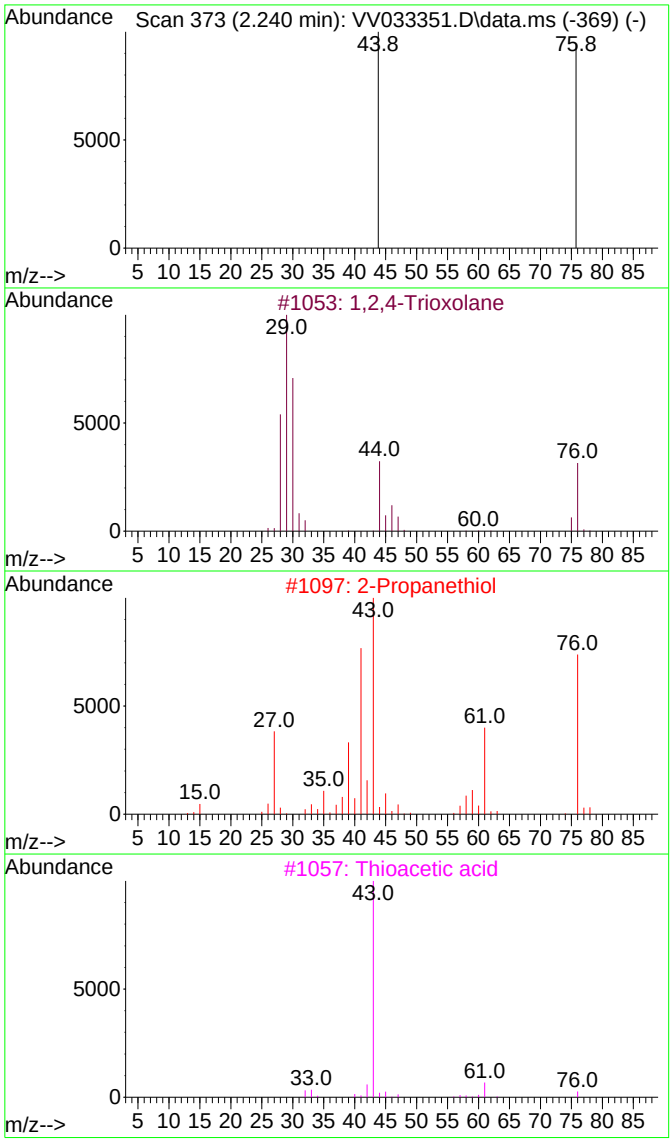
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

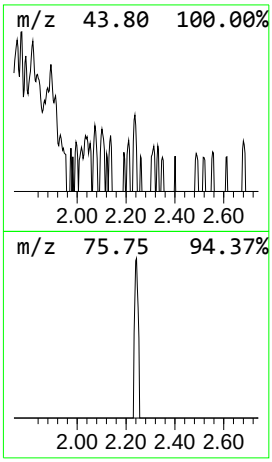
****

Peak Number 2 unknown-02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.240	123.94 ug/L	352	1,4-Difluorobenzene	5.535

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Trioxolane	76	C2H4O3	000289-14-5	4
2	2-Propanethiol	76	C3H8S	000075-33-2	3
3	Thioacetic acid	76	C2H4OS	000507-09-5	2
4	2-Propanethiol	76	C3H8S	000075-33-2	2
5	2-Propanethiol	76	C3H8S	000075-33-2	2





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121423\
Data File : VV033351.D
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ALS Vial : 30 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AX8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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

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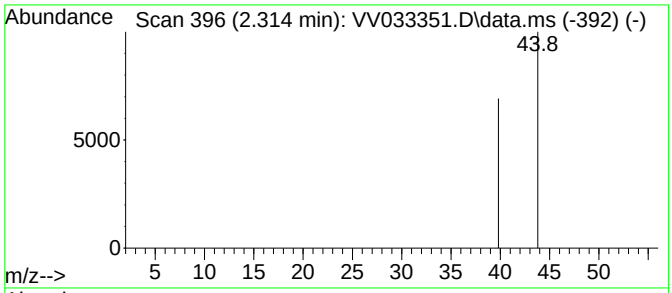
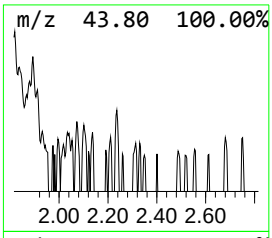
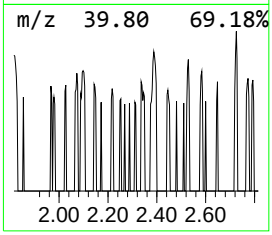
Peak Number 3 unknown-03 Concentration Rank 14

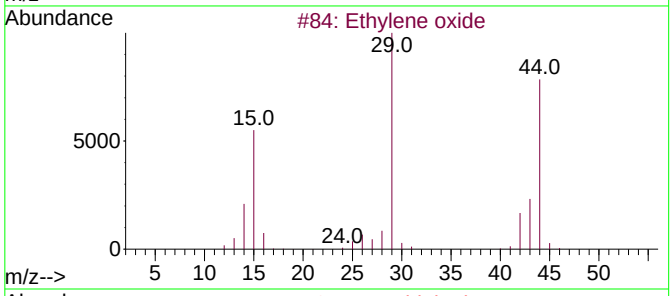
R.T.	EstConc	Area	Relative to ISTD	R.T.
2.314	56.69 ug/L	161	1,4-Difluorobenzene	5.535

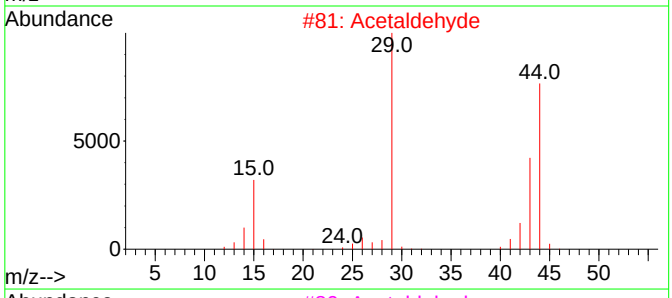
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethylene oxide	44	C2H4O	000075-21-8	2
2	Acetaldehyde	44	C2H4O	000075-07-0	2
3	Acetaldehyde	44	C2H4O	000075-07-0	2
4	Acetonitrile-d3	44	C2D3N	002206-26-0	2
5	Acetonitrile-d3	44	C2D3N	002206-26-0	2

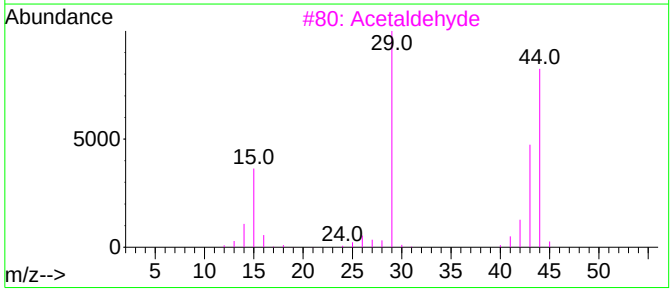












Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121423\
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ALS Vial : 30 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AX8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

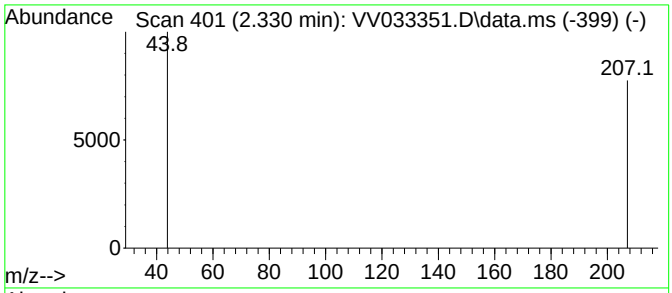
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

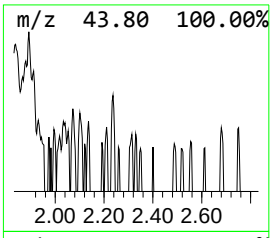
****

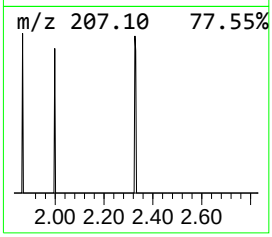
Peak Number 4 unknown-04 Concentration Rank 16

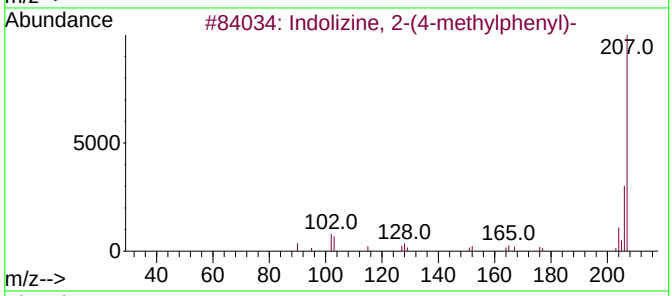
R.T.	EstConc	Area	Relative to ISTD	R.T.
2.330	51.06 ug/L	145	1,4-Difluorobenzene	5.535

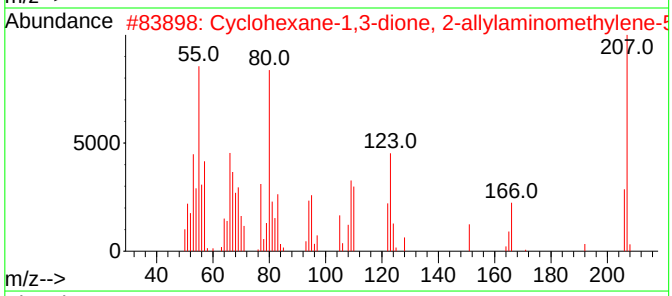
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indolizine, 2-(4-methylphenyl)-	207	C15H13N	007496-81-3	2
2	Cyclohexane-1,3-dione, 2-allylam...	207	C12H17NO2	104926-37-6	2
3	6-Nitro-8-methoxy-2H-chromene	207	C10H9NO4	062063-07-4	2
4	MDMA methylene homolog	207	C12H17NO2	1010386-32-2	2
5	Ethyl 5-(furan-2-yl)-1,2-oxazole...	207	C10H9NO4	1000411-40-9	2

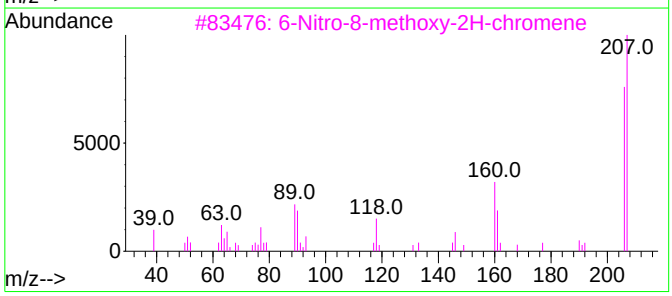












Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121423\
Data File : VV033351.D
Acq On : 14 Dec 2023 21:46
Operator : SY/MD
Sample : 05807-06 100X
Misc : 2.55g/5.0mL/100uL/5.00mL/MSVOA_V/MEOH
ALS Vial : 30 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AX8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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

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Peak Number 6 unknown-05 Concentration Rank 27

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.487	36.97 ug/L	105	1,4-Difluorobenzene	5.535

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyne, fluoro-	44	C2HF	002713-09-9	2
2	Acetaldehyde	44	C2H4O	000075-07-0	2
3	Acetonitrile-d3	44	C2D3N	002206-26-0	2
4	Ethylene oxide	44	C2H4O	000075-21-8	2
5	Nitrous oxide	44	N2O	010024-97-2	2