

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV092524\
 Data File : VV037516.D
 Acq On : 25 Sep 2024 12:11
 Operator : SY/MD
 Sample : P4109-14ME
 Misc : 5.05G/5.0mL/100uL/5mL/MSVOA_V/MEOH
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 A4ET6ME

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\SFAMVLM082624WMA.M
 Title : VOC Analysis

Signal : TIC: VV037516.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.182	34	44	50	rBV2	21896	43602	1.85%	0.240%
2	1.278	67	74	90	rVB	235934	290474	12.35%	1.597%
3	1.503	107	144	169	rBV2	165484	513588	21.84%	2.824%
4	2.043	303	312	327	rBV	493306	702621	29.87%	3.863%
5	2.371	406	414	426	rBV2	35643	60330	2.57%	0.332%
6	3.268	690	693	699	rVB4	1214	1093	0.05%	0.006%
7	3.378	724	727	731	rVB4	996	684	0.03%	0.004%
8	3.539	775	777	781	rVV4	761	607	0.03%	0.003%
9	3.584	787	791	793	rBV2	704	559	0.02%	0.003%
10	3.648	807	811	813	rBV3	755	653	0.03%	0.004%
11	3.719	829	833	838	rBV6	837	1081	0.05%	0.006%
12	3.799	847	858	895	rBV2	99932	338284	14.38%	1.860%
13	4.239	976	995	1024	rBV	371689	955261	40.61%	5.252%
14	4.696	1133	1137	1142	rVB5	1033	1014	0.04%	0.006%
15	4.850	1181	1185	1189	rVB3	652	547	0.02%	0.003%
16	4.944	1196	1214	1249	rBV2	933927	2352001	100.00%	12.932%
17	5.198	1287	1293	1297	rBV8	1544	1532	0.07%	0.008%
18	5.259	1308	1312	1313	rBV3	969	573	0.02%	0.003%
19	5.384	1348	1351	1354	rBV4	1039	773	0.03%	0.004%
20	5.403	1354	1357	1360	rVV5	1147	770	0.03%	0.004%
21	5.468	1370	1377	1380	rBV7	912	916	0.04%	0.005%
22	5.526	1382	1395	1433	rBV	747426	1563333	66.47%	8.595%
23	5.818	1479	1486	1487	rBV5	5205	4560	0.19%	0.025%
24	5.921	1512	1518	1520	rBV5	1696	1726	0.07%	0.009%
25	5.934	1520	1522	1524	rVV3	1104	672	0.03%	0.004%
26	5.982	1524	1537	1567	rVV	513705	1071638	45.56%	5.892%
27	6.255	1620	1622	1627	rVB4	1212	1086	0.05%	0.006%
28	6.374	1656	1659	1664	rBV4	1082	1189	0.05%	0.007%
29	6.519	1700	1704	1708	rVB5	976	904	0.04%	0.005%
30	6.593	1722	1727	1733	rBV7	780	743	0.03%	0.004%
31	6.645	1741	1743	1747	rVB3	1065	634	0.03%	0.003%
32	6.670	1747	1751	1753	rBV4	1164	1100	0.05%	0.006%
33	6.908	1814	1825	1854	rBV	275042	535456	22.77%	2.944%
34	7.101	1883	1885	1888	rVB4	1142	634	0.03%	0.003%
35	7.236	1915	1927	1963	rBV	1019453	1825389	77.61%	10.036%
36	7.480	2000	2003	2006	rBV4	1285	981	0.04%	0.005%

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Integrator: RTE

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
 Title : VOC Analysis

37	7.548	2015	2024	2053	rBV	184475	350108	14.89%	1.925%
38	7.860	2116	2121	2122	rBV3	1696	1246	0.05%	0.007%
39	7.947	2145	2148	2151	rVB3	844	646	0.03%	0.004%
40	8.027	2164	2173	2211	rBV	356758	748457	31.82%	4.115%
41	8.361	2273	2277	2286	rVB6	2942	4431	0.19%	0.024%
42	8.779	2395	2407	2441	rBV	1168323	1962106	83.42%	10.788%
43	8.934	2453	2455	2457	rBV3	1269	550	0.02%	0.003%
44	9.101	2505	2507	2510	rBV3	744	570	0.02%	0.003%
45	9.451	2613	2616	2621	rVB5	978	620	0.03%	0.003%
46	9.680	2684	2687	2690	rVB4	991	580	0.02%	0.003%
47	9.779	2714	2718	2724	rVB5	965	1089	0.05%	0.006%
48	9.812	2724	2728	2729	rBV2	960	637	0.03%	0.004%
49	9.908	2748	2758	2760	rBV7	2023	2342	0.10%	0.013%
50	9.934	2764	2766	2769	rVB4	1481	719	0.03%	0.004%
51	10.146	2821	2832	2858	rVV	616670	989161	42.06%	5.438%
52	10.313	2882	2884	2887	rBV4	1091	682	0.03%	0.004%
53	10.374	2901	2903	2906	rVB3	912	540	0.02%	0.003%
54	10.480	2932	2936	2941	rVB5	759	797	0.03%	0.004%
55	10.513	2941	2946	2947	rBV3	817	726	0.03%	0.004%
56	10.545	2954	2956	2960	rVB4	827	553	0.02%	0.003%
57	10.609	2972	2976	2980	rVB4	880	722	0.03%	0.004%
58	10.731	3010	3014	3016	rBV4	730	543	0.02%	0.003%
59	10.750	3016	3020	3024	rBV5	1865	1578	0.07%	0.009%
60	10.792	3029	3033	3036	rBV6	1559	903	0.04%	0.005%
61	10.853	3048	3052	3055	rBV3	1305	920	0.04%	0.005%
62	10.905	3064	3068	3074	rVB4	729	667	0.03%	0.004%
63	10.950	3078	3082	3085	rVB3	964	688	0.03%	0.004%
64	11.127	3127	3137	3139	rBV6	1795	2142	0.09%	0.012%
65	11.178	3141	3153	3181	rBV	1248499	1974914	83.97%	10.858%
66	11.554	3258	3270	3296	rBV	1114664	1777911	75.59%	9.775%
67	11.773	3333	3338	3342	rBV5	1747	1975	0.08%	0.011%
68	11.934	3384	3388	3393	rVB6	1309	1053	0.04%	0.006%
69	12.004	3406	3410	3412	rBV3	999	636	0.03%	0.003%
70	12.056	3423	3426	3429	rBV3	872	637	0.03%	0.004%
71	12.162	3456	3459	3461	rBV4	1012	580	0.02%	0.003%
72	12.188	3461	3467	3474	rVB6	2208	2787	0.12%	0.015%
73	12.332	3501	3512	3523	rVV9	5703	15124	0.64%	0.083%
74	12.519	3568	3570	3574	rBV4	925	825	0.04%	0.005%
75	12.570	3581	3586	3587	rBV4	1433	1290	0.05%	0.007%
76	12.824	3660	3665	3671	rBV8	1046	1146	0.05%	0.006%

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 ClientSampleId :
 A4ET6ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
 Title : VOC Analysis

77	12.860	3671	3676	3681	rVB6	1481	1221	0.05%	0.007%
78	12.885	3681	3684	3686	rBV4	756	644	0.03%	0.004%
79	12.966	3706	3709	3711	rBV4	1081	732	0.03%	0.004%
80	13.011	3716	3723	3733	rBV9	8790	15668	0.67%	0.086%
81	13.101	3749	3751	3755	rBV3	891	788	0.03%	0.004%
82	13.155	3762	3768	3771	rBV5	1308	1467	0.06%	0.008%
83	13.217	3783	3787	3788	rBV4	1712	1218	0.05%	0.007%
84	13.384	3834	3839	3846	rBV10	3436	4568	0.19%	0.025%
85	13.496	3872	3874	3877	rBV3	1469	763	0.03%	0.004%
86	13.641	3913	3919	3923	rBV4	1464	1559	0.07%	0.009%
87	13.664	3923	3926	3928	rBV3	1437	849	0.04%	0.005%
88	13.689	3932	3934	3938	rVV5	1152	699	0.03%	0.004%
89	13.795	3963	3967	3970	rBV6	1454	1192	0.05%	0.007%
90	13.975	4020	4023	4026	rBV5	934	818	0.03%	0.004%
91	14.024	4036	4038	4041	rVB3	1525	843	0.04%	0.005%
92	14.075	4052	4054	4057	rVB3	1751	729	0.03%	0.004%
93	14.217	4096	4098	4100	rBV3	1373	644	0.03%	0.004%
94	14.303	4119	4125	4126	rBV6	1502	1540	0.07%	0.008%
95	14.364	4137	4144	4150	rBV8	4761	7630	0.32%	0.042%
96	14.519	4189	4192	4194	rBV3	1944	1223	0.05%	0.007%
97	14.570	4204	4208	4210	rBV4	1597	1461	0.06%	0.008%
98	14.708	4249	4251	4254	rBV4	1823	1276	0.05%	0.007%
99	14.927	4317	4319	4322	rBV5	1818	1135	0.05%	0.006%
100	14.959	4322	4329	4335	rVV10	5407	8859	0.38%	0.049%

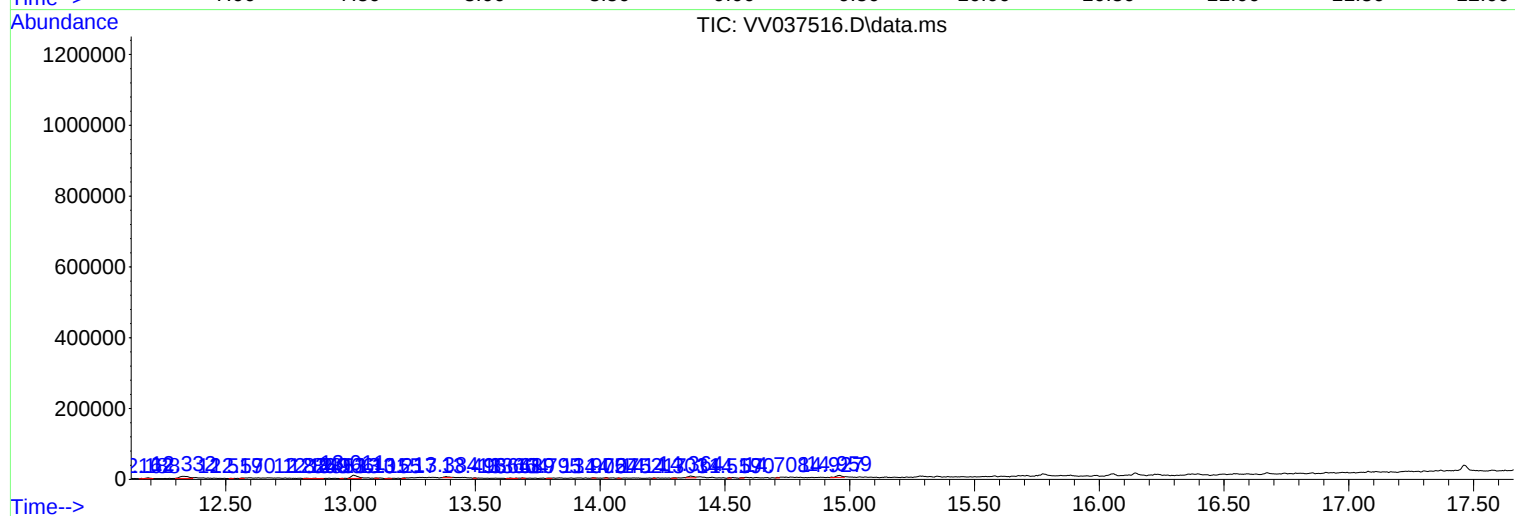
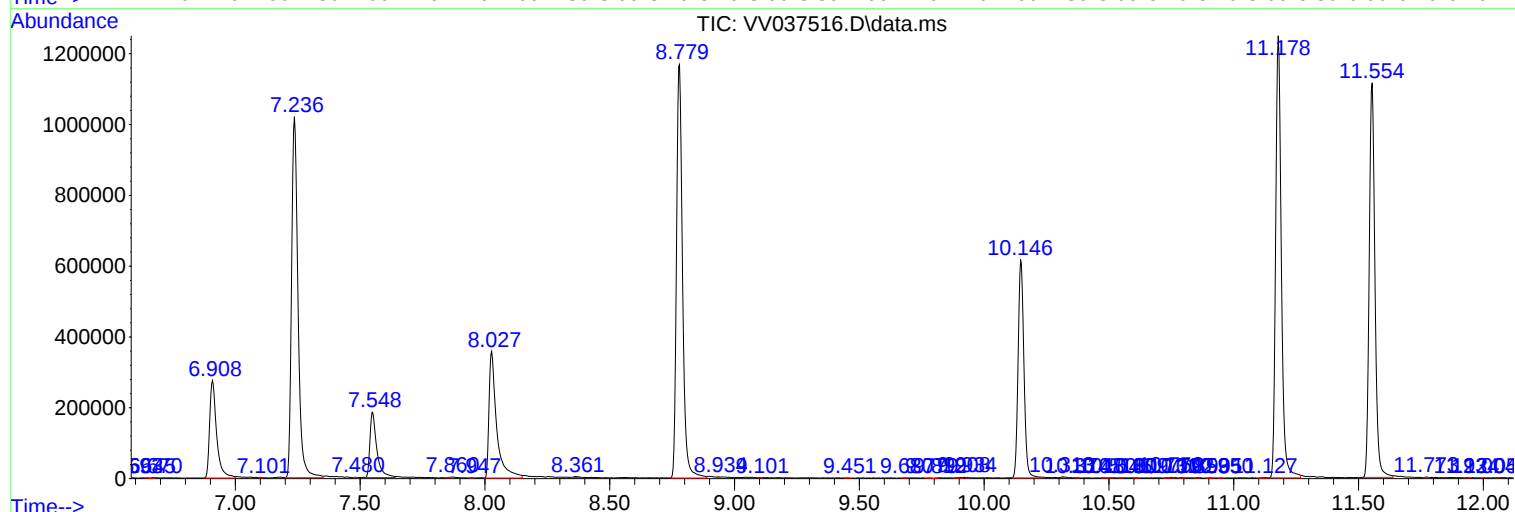
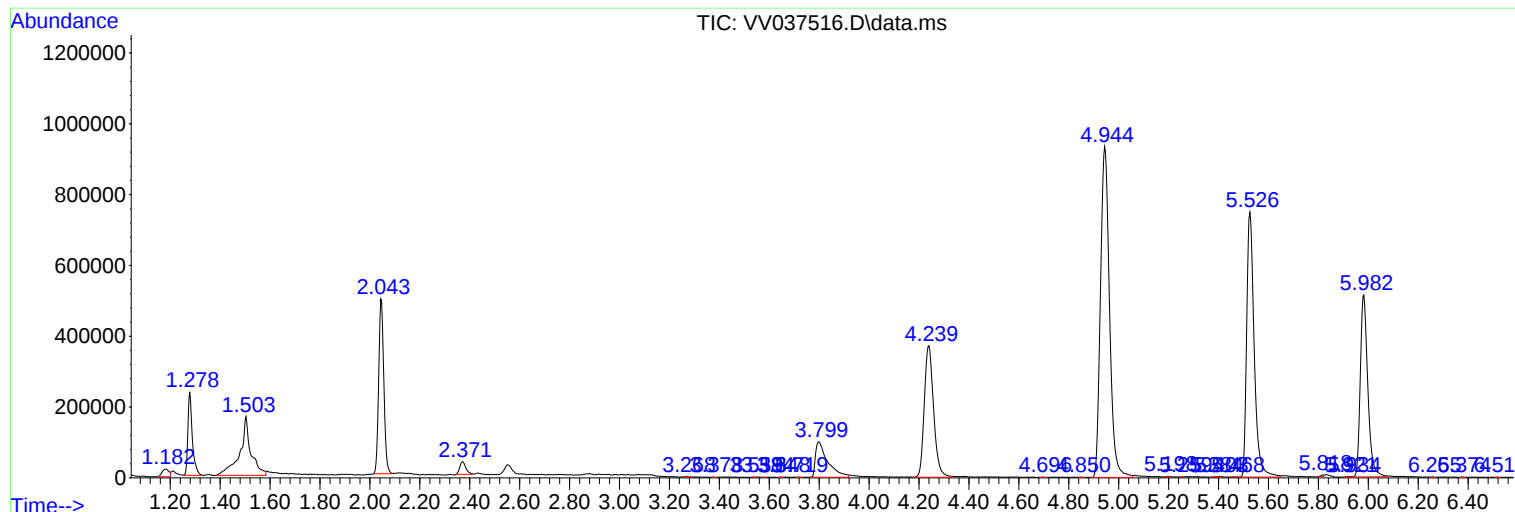
Sum of corrected areas: 18188135

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Instrument :
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ClientSampleId :
A4ET6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
A4ET6ME

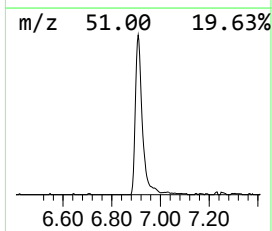
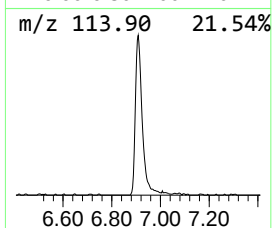
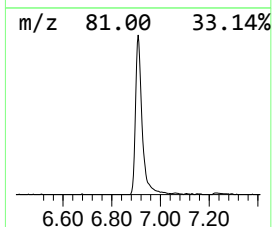
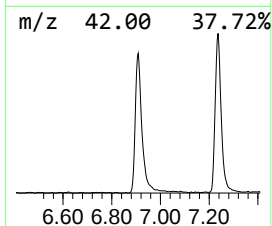
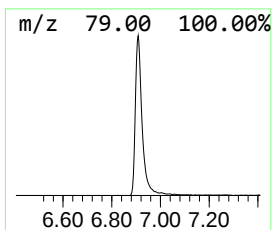
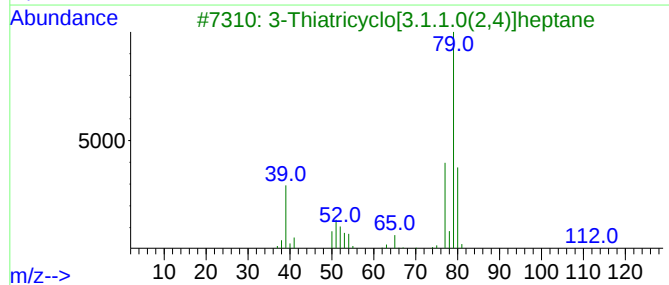
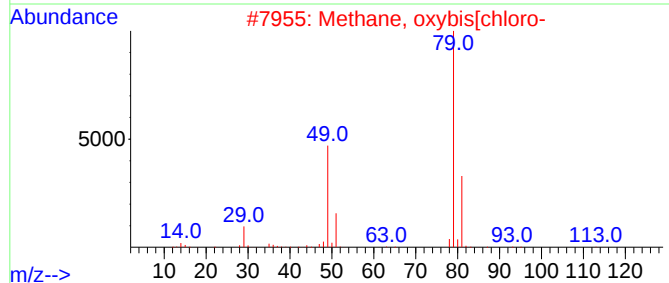
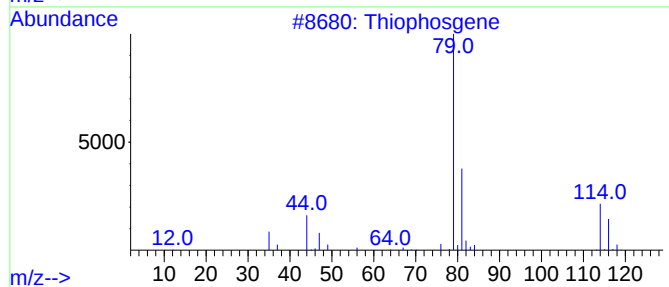
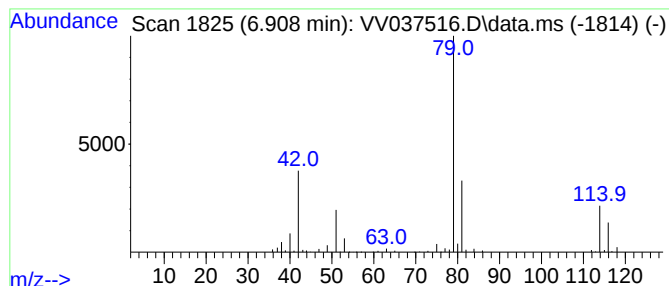
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Thiophosgene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.908	17.13 ug/L	535456	1,4-Difluorobenzene	5.526

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophosgene	114	CCl2S	000463-71-8	58
2			Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	40
3			3-Thiatricyclo[3.1.1.0(2,4)]heptane	112	C6H8S	1000221-37-0	38
4			1,3-Cyclohexadiene	80	C6H8	000592-57-4	28
5			2-Propanol, 1,3-dichloro-	128	C3H6Cl2O	000096-23-1	28



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Thiophosgene	6.908	17.1	ug/L	535456	1	5.526	1563330	50.0