

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV041824\
 Data File : VV035287.D
 Acq On : 18 Apr 2024 16:50
 Operator : SY/MD
 Sample : P2158-11
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 MCORE1

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
 Title : VOC Analysis

Signal : TIC: VV035287.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.085	10	14	24	rVB9	2344	3178	0.00%	0.000%
2	1.188	40	46	49	rBV2	3560	3426	0.00%	0.000%
3	1.217	49	55	60	rBV	4831	6196	0.00%	0.000%
4	1.278	67	74	89	rBV	209444	225024	0.06%	0.017%
5	1.384	102	107	113	rBV2	4419	4761	0.00%	0.000%
6	1.449	116	127	129	rBV7	9471	15732	0.00%	0.001%
7	1.478	131	136	137	rBV4	5212	4279	0.00%	0.000%
8	1.523	144	150	165	rVB	180998	222770	0.06%	0.017%
9	2.056	305	316	329	rBV	358256	519634	0.13%	0.039%
10	2.243	362	374	378	rBV8	2929	4907	0.00%	0.000%
11	2.400	419	423	424	rBV2	463	312	0.00%	0.000%
12	2.449	428	438	442	rBV6	2876	5100	0.00%	0.000%
13	2.561	459	473	499	rVB2	28875	78246	0.02%	0.006%
14	2.696	504	515	528	rVB9	3240	6985	0.00%	0.001%
15	2.883	566	573	574	rBV3	749	728	0.00%	0.000%
16	2.966	594	599	601	rBV2	1074	1028	0.00%	0.000%
17	3.037	617	621	625	rVB4	333	318	0.00%	0.000%
18	3.111	641	644	646	rBV3	525	418	0.00%	0.000%
19	3.442	743	747	752	rVB3	374	330	0.00%	0.000%
20	3.667	798	817	844	rBV2	85787	221838	0.06%	0.017%
21	3.789	844	855	899	rBV2	130193	426556	0.11%	0.032%
22	4.246	980	997	1031	rBV	255402	658583	0.17%	0.050%
23	4.580	1082	1101	1124	rVB3	53695	140784	0.04%	0.011%
24	4.735	1130	1149	1168	rBV4	44681	110936	0.03%	0.008%
25	4.834	1170	1180	1181	rBV5	1539	1876	0.00%	0.000%
26	4.847	1181	1184	1197	rVB8	3177	4981	0.00%	0.000%
27	4.953	1200	1217	1228	rBV2	621925	1614813	0.41%	0.123%
28	5.156	1275	1280	1282	rBV6	2192	2052	0.00%	0.000%
29	5.240	1295	1306	1316	rVB9	4365	10143	0.00%	0.001%
30	5.359	1337	1343	1346	rVB6	793	604	0.00%	0.000%
31	5.394	1350	1354	1355	rBV3	466	354	0.00%	0.000%
32	5.416	1355	1361	1364	rVB4	588	637	0.00%	0.000%
33	5.432	1364	1366	1372	rVB2	463	395	0.00%	0.000%
34	5.458	1372	1374	1376	rVB2	728	404	0.00%	0.000%
35	5.474	1376	1379	1380	rBV2	704	402	0.00%	0.000%
36	5.535	1383	1398	1433	rBV	360232	773422	0.20%	0.059%

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
 Title : VOC Analysis

37	5.703	1448	1450	1453	rVB4	751	360	0.00%	0.000%
38	5.719	1453	1455	1460	rVV3	603	420	0.00%	0.000%
39	5.838	1486	1492	1493	rBV2	1157	1136	0.00%	0.000%
40	5.850	1494	1496	1501	rVB4	855	505	0.00%	0.000%
41	5.870	1501	1502	1505	rVB2	1639	538	0.00%	0.000%
42	5.989	1523	1539	1572	rBV	356365	839340	0.21%	0.064%
43	6.159	1588	1592	1600	rVB6	914	1243	0.00%	0.000%
44	6.217	1607	1610	1612	rVV3	668	373	0.00%	0.000%
45	6.288	1622	1632	1645	rVV6	4794	10566	0.00%	0.001%
46	6.445	1674	1681	1685	rVB3	669	754	0.00%	0.000%
47	6.471	1685	1689	1692	rBV3	527	381	0.00%	0.000%
48	6.632	1736	1739	1742	rBV3	576	393	0.00%	0.000%
49	6.651	1742	1745	1750	rVB3	409	412	0.00%	0.000%
50	6.674	1750	1752	1755	rVB2	805	375	0.00%	0.000%
51	6.719	1755	1766	1768	rBV8	2973	4157	0.00%	0.000%
52	6.776	1782	1784	1792	rVB4	504	487	0.00%	0.000%
53	6.915	1815	1827	1853	rBV	178741	358584	0.09%	0.027%
54	7.156	1894	1902	1906	rBV8	885	1257	0.00%	0.000%
55	7.246	1916	1930	1948	rBV	671641	1270768	0.32%	0.096%
56	7.326	1949	1955	1975	rVB	31821	70725	0.02%	0.005%
57	7.558	2016	2027	2060	rBV	126404	252976	0.06%	0.019%
58	7.757	2085	2089	2092	rVB4	543	404	0.00%	0.000%
59	7.773	2092	2094	2100	rVB4	838	753	0.00%	0.000%
60	7.802	2100	2103	2106	rBV3	760	482	0.00%	0.000%
61	7.911	2119	2137	2154	rBV3	24613	52549	0.01%	0.004%
62	8.040	2164	2177	2215	rBV2	343076	829003	0.21%	0.063%
63	8.391	2284	2286	2290	rVB3	673	505	0.00%	0.000%
64	8.532	2327	2330	2335	rVB4	319	322	0.00%	0.000%
65	8.841	2399	2426	2448	rBV7	71145025	392219231	100.00%	29.775%
66	8.924	2450	2452	2495	rVB3	57925204	43295708	11.04%	3.287%
67	10.156	2823	2835	2863	rBV2	805261	1331496	0.34%	0.101%
68	10.326	2884	2888	2893	rBV4	2613	2879	0.00%	0.000%
69	10.368	2893	2901	2920	rVB	42421	75902	0.02%	0.006%
70	10.490	2930	2939	2955	rBV	20672	41564	0.01%	0.003%
71	10.635	2980	2984	2985	rBV4	650	439	0.00%	0.000%
72	10.677	2995	2997	2998	rBV2	711	342	0.00%	0.000%
73	10.786	3028	3031	3033	rBV4	584	329	0.00%	0.000%
74	10.802	3033	3036	3037	rBV2	953	517	0.00%	0.000%
75	10.870	3048	3057	3069	rBV3	6974	12547	0.00%	0.001%
76	10.963	3082	3086	3090	rBV4	1042	870	0.00%	0.000%

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
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77	11.130	3120	3138	3152	rBV	37383819	75923888	19.36%	5.764%
78	11.233	3152	3170	3192	rVB5	70472730	198582582	50.63%	15.075%
79	11.606	3264	3286	3306	rBV8	71151073	339981110	86.68%	25.809%
80	11.680	3307	3309	3371	rVB	55105625	39210199	10.00%	2.977%
81	12.056	3419	3426	3442	rVB2	33912	58106	0.01%	0.004%
82	12.281	3486	3496	3502	rVB2	33290	54800	0.01%	0.004%
83	12.336	3502	3513	3535	rVB	2026487	3048813	0.78%	0.231%
84	12.522	3558	3571	3585	rBV3	184538	449609	0.11%	0.034%
85	12.590	3585	3592	3606	rVB2	40560	68429	0.02%	0.005%
86	12.686	3611	3622	3646	rVB	797210	1284684	0.33%	0.098%
87	12.828	3663	3666	3676	rVB9	3495	4188	0.00%	0.000%
88	12.937	3690	3700	3717	rBV3	36495	74228	0.02%	0.006%
89	13.223	3767	3789	3836	rBV3	68581547	173042136	44.12%	13.136%
90	13.445	3848	3858	3879	rVB	208990	339348	0.09%	0.026%
91	13.686	3917	3933	3961	rBV	24757138	37547165	9.57%	2.850%
92	14.236	4093	4104	4125	rVB5	20649	48004	0.01%	0.004%
93	14.448	4164	4170	4181	rVB5	7143	10707	0.00%	0.001%
94	14.551	4195	4202	4207	rBV3	11416	17600	0.00%	0.001%
95	14.757	4242	4266	4288	rBV	337742	621767	0.16%	0.047%
96	14.943	4318	4324	4333	rVB7	4088	6471	0.00%	0.000%
97	15.226	4410	4412	4416	rBV3	875	511	0.00%	0.000%
98	15.332	4433	4445	4470	rBV	725845	1161269	0.30%	0.088%
99	15.831	4597	4600	4602	rBV4	1165	868	0.00%	0.000%
100	16.207	4715	4717	4719	rBV3	1194	578	0.00%	0.000%

Sum of corrected areas: 1317290804

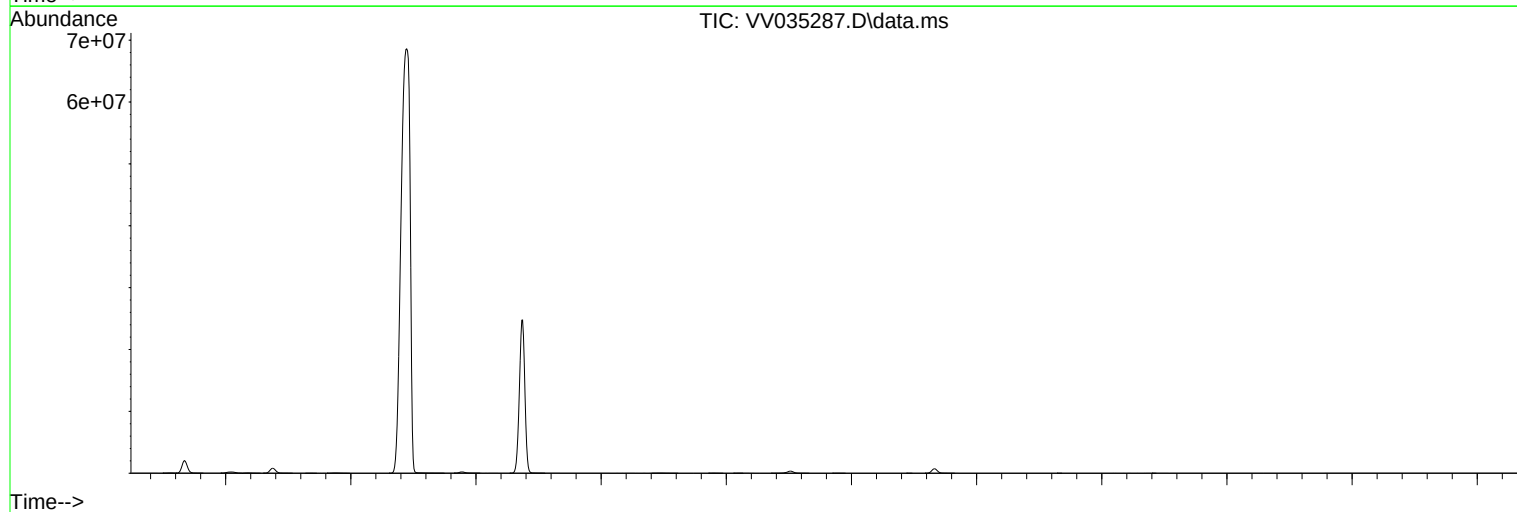
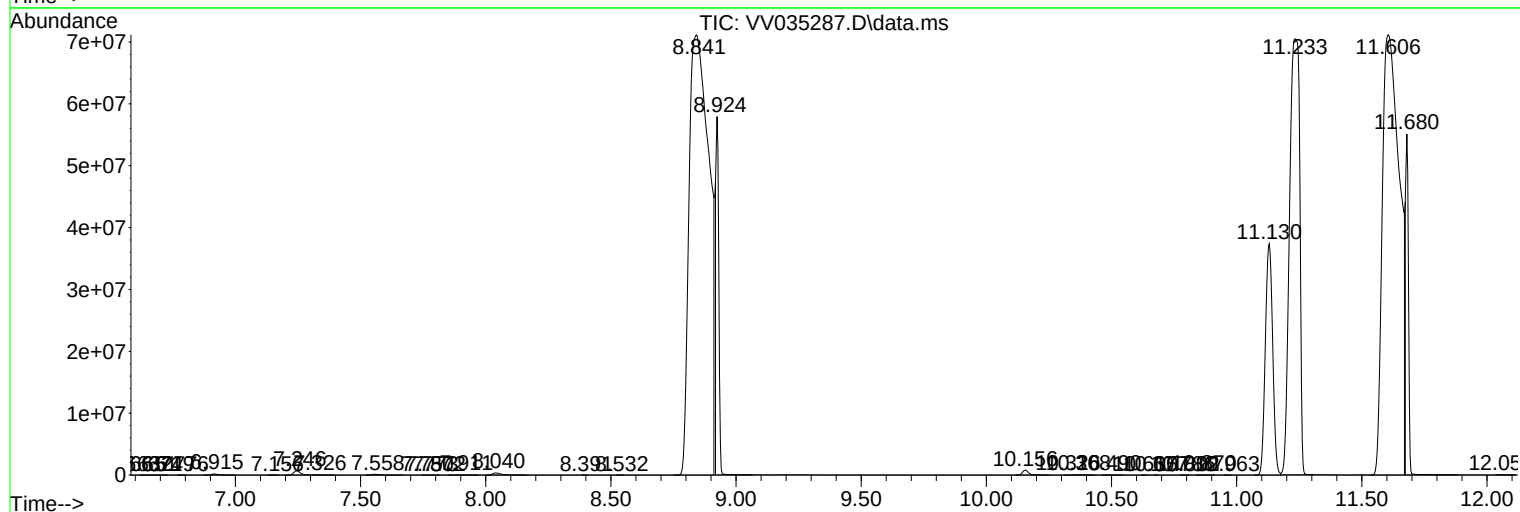
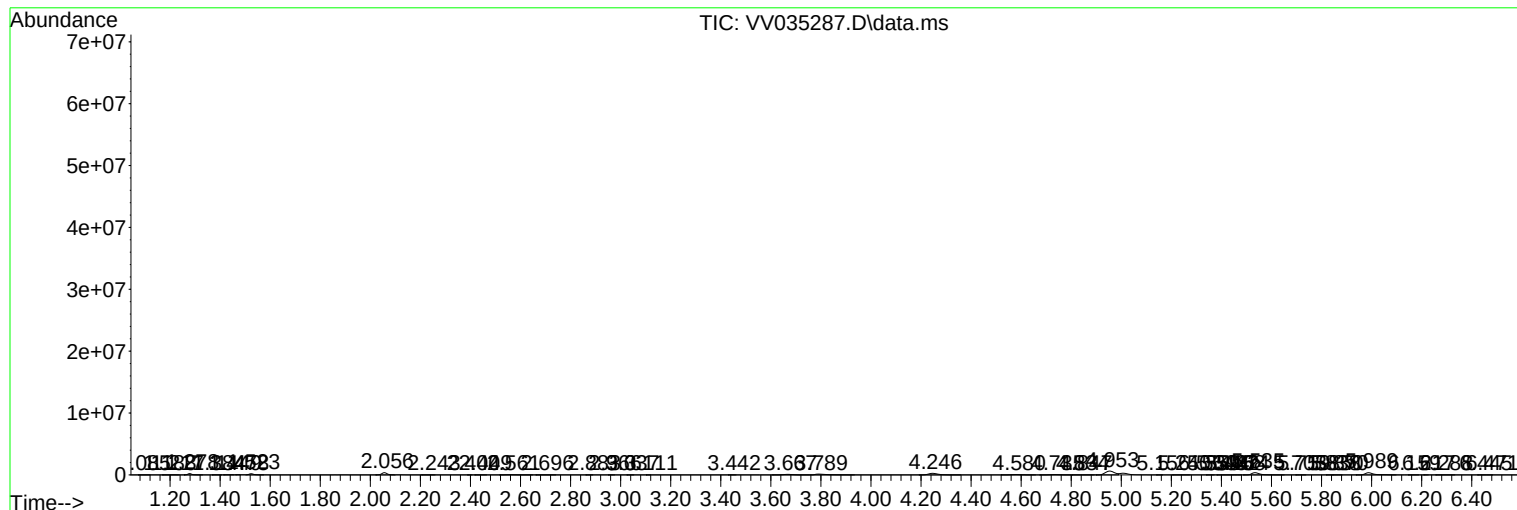
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
MCORE1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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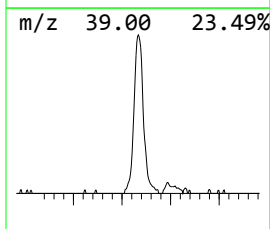
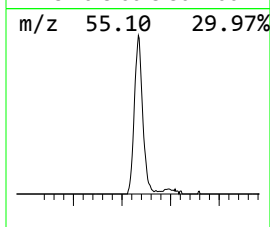
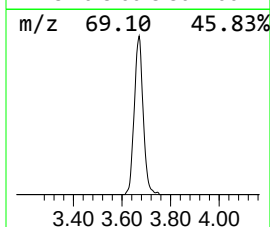
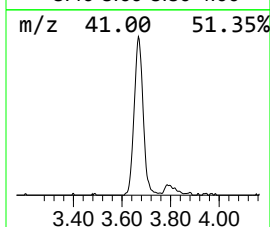
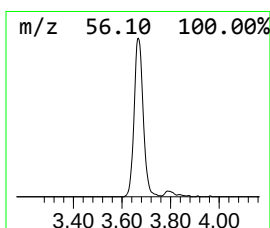
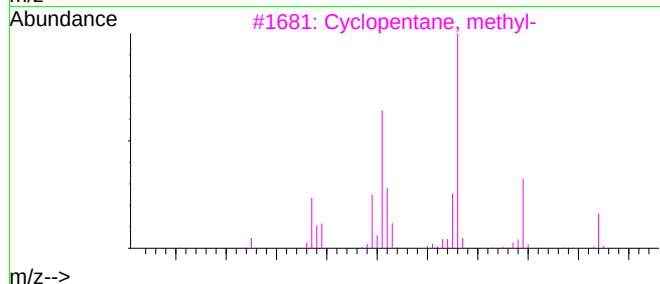
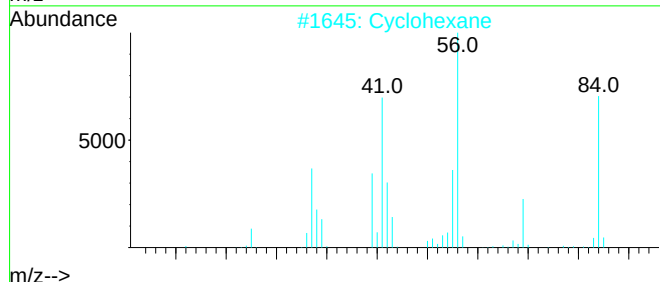
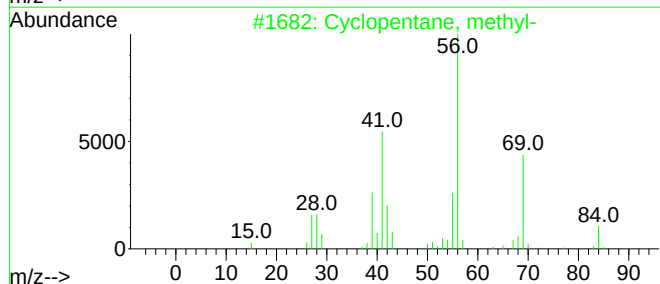
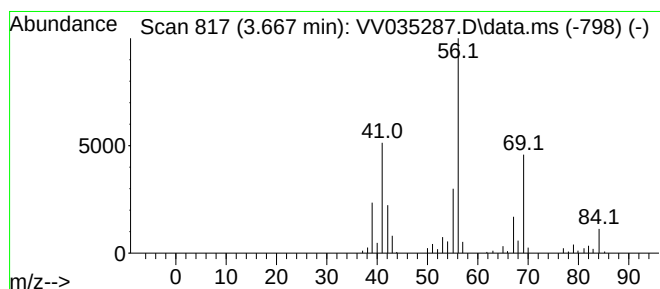
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 2 (DEL) Alkane: Cyclic3.667 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
3.667	14.34 ug/L	221838	1,4-Difluorobenzene	5.535	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	87
2	Cyclohexane	84	C6H12	000110-82-7	74
3	Cyclopentane, methyl-	84	C6H12	000096-37-7	72
4	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	72
5	Cyclohexane	84	C6H12	000110-82-7	72



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Quant Title : VOC Analysis

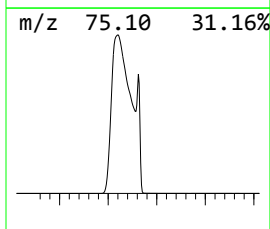
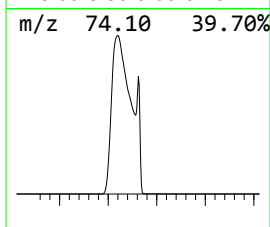
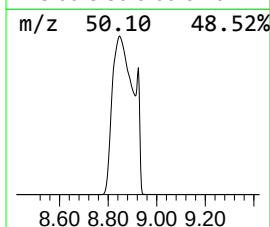
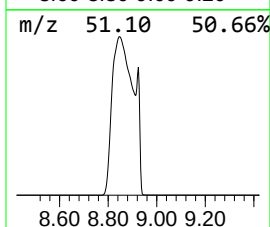
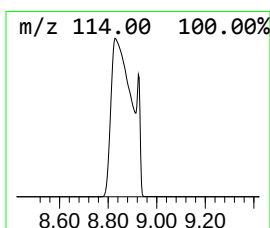
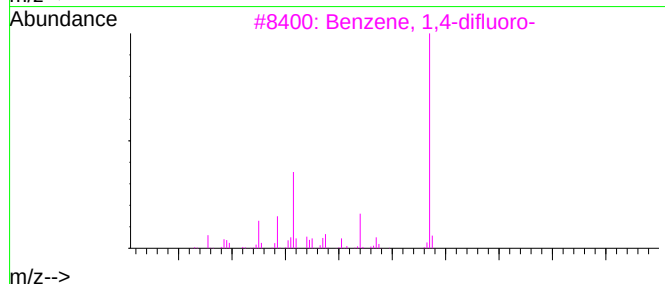
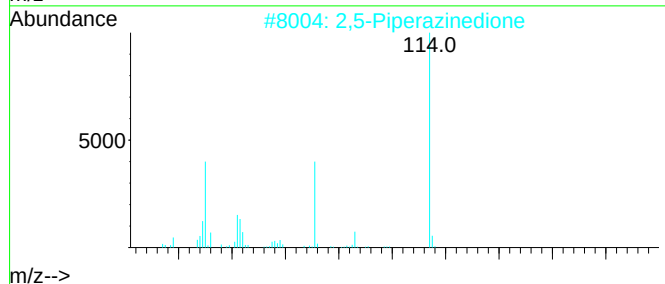
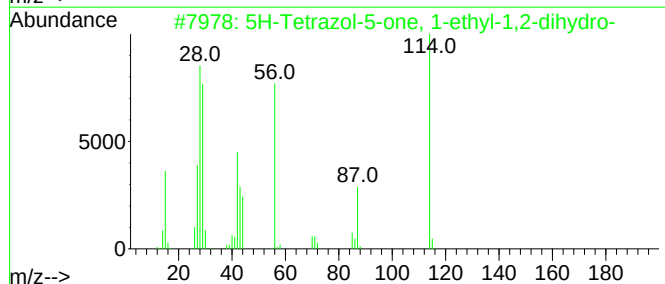
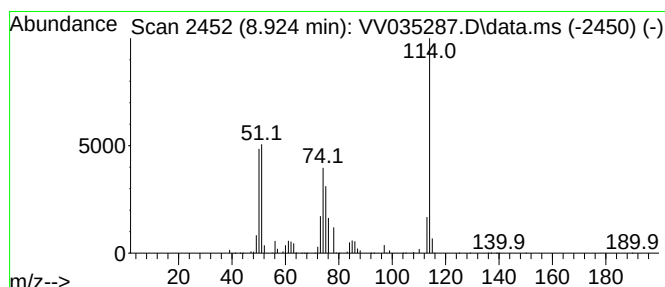
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.924	5.52 ug/L	43295700	Chlorobenzene-d5	8.825

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Tetrazol-5-one, 1-ethyl-1,2-d...	114	C3H6N4O	069048-98-2	10
2	2,5-Piperazinedione	114	C4H6N2O2	000106-57-0	9
3	Benzene, 1,4-difluoro-	114	C6H4F2	000540-36-3	9
4	2-p-Nitrobenzoyl-1,3,5-tribenzyl...	569	C33H31NO8	1000129-85-6	9
5	3-Amino-2-hydroxyheptanoic acid,...	217	C11H23NO3	1000501-26-5	9



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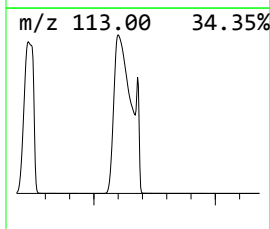
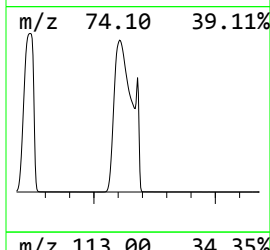
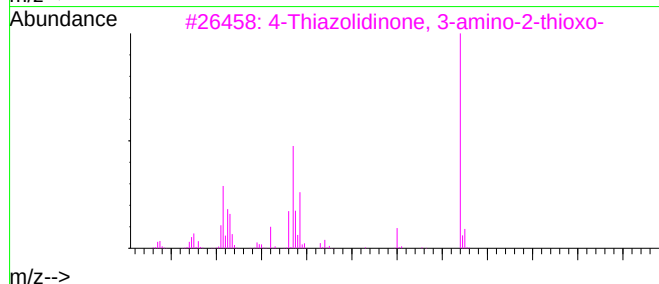
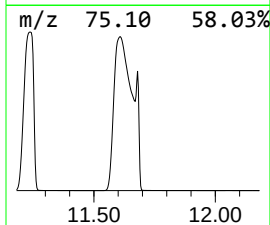
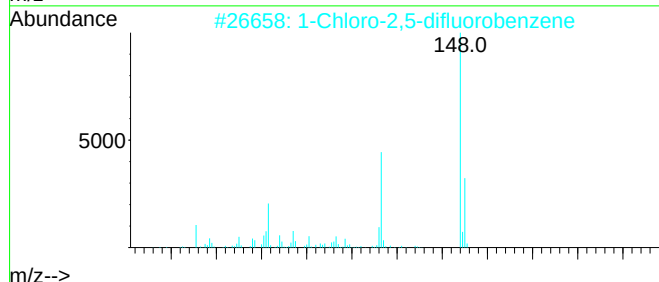
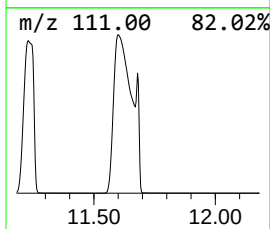
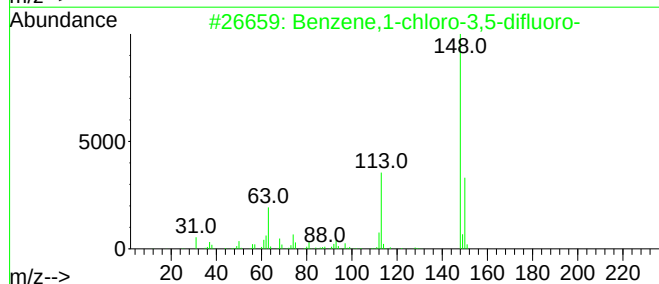
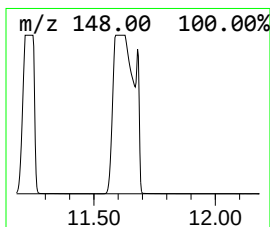
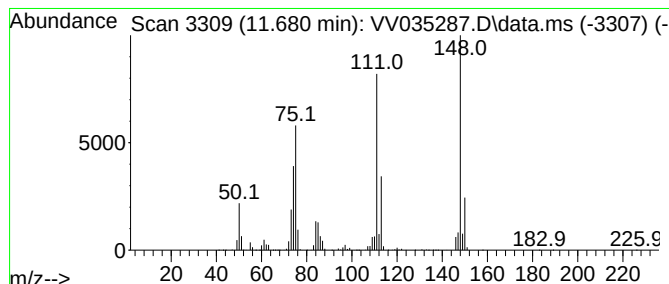
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown-02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.680	9.87 ug/L	39210200	1,4-Dichlorobenzene-d4	11.204	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene,1-chloro-3,5-difluoro-	148	C6H3ClF2	001435-43-4	25
2	1-Chloro-2,5-difluorobenzene	148	C6H3ClF2	002367-91-1	22
3	4-Thiazolidinone, 3-amino-2-thioxo-	148	C3H4N2OS2	001438-16-0	17
4	3-Chloro-4-nitroisoxazole	148	C3HClN2O3	1000432-93-0	16
5	1-Chloro-2,4-difluorobenzene	148	C6H3ClF2	001435-44-5	12



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV041824\
Data File : VV035287.D
Acq On : 18 Apr 2024 16:50
Operator : SY/MD
Sample : P2158-11
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
MCORE1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: C...	3.667	14.3	ug/L	221838	1	5.535	773422	50.0
unknown-01	8.924	5.5	ug/L	43295700	2	8.825	392219000	50.0
unknown-02	11.680	9.9	ug/L	39210200	3	11.204	198583000	50.0