

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042822\
 Data File : VU048340.D
 Acq On : 28 Apr 2022 14:50
 Operator : SY/MD
 Sample : N2587-10DL 40X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXET6DL

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: VU048340.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.359	3	6	26	rVB	4794953	4664919	100.00%	22.170%
2	1.436	27	30	39	rVB2	6244	5716	0.12%	0.027%
3	1.523	52	57	67	rBV3	5656	9526	0.20%	0.045%
4	1.600	73	81	102	rBV	166800	223347	4.79%	1.061%
5	1.906	169	176	208	rVB	148852	255616	5.48%	1.215%
6	2.469	347	351	353	rBV3	888	756	0.02%	0.004%
7	2.565	369	381	395	rBV	326150	534631	11.46%	2.541%
8	2.639	396	404	413	rBV	32181	58536	1.25%	0.278%
9	3.134	546	558	566	rBV2	29834	61650	1.32%	0.293%
10	3.308	610	612	616	rVB3	704	501	0.01%	0.002%
11	3.350	619	625	628	rBV5	819	923	0.02%	0.004%
12	3.446	643	655	666	rVB7	2078	4486	0.10%	0.021%
13	3.514	670	676	679	rVV2	405	454	0.01%	0.002%
14	3.700	726	734	741	rVB3	1065	1560	0.03%	0.007%
15	3.854	776	782	784	rBV	952	987	0.02%	0.005%
16	4.076	845	851	856	rBV2	392	373	0.01%	0.002%
17	4.250	896	905	917	rBV5	1022	1934	0.04%	0.009%
18	4.459	964	970	975	rVB3	413	534	0.01%	0.003%
19	4.530	975	992	994	rBV5	1247	2416	0.05%	0.011%
20	4.632	1010	1024	1046	rBV	194937	532114	11.41%	2.529%
21	4.973	1128	1130	1136	rVB3	482	393	0.01%	0.002%
22	5.063	1136	1158	1181	rBV	303908	667849	14.32%	3.174%
23	5.388	1249	1259	1274	rVB8	2296	5279	0.11%	0.025%
24	5.726	1342	1364	1371	rBV2	633070	1667508	35.75%	7.925%
25	5.774	1373	1379	1407	rVB	771571	1448157	31.04%	6.882%
26	5.970	1435	1440	1445	rBV6	1310	1475	0.03%	0.007%
27	6.137	1488	1492	1494	rBV3	781	526	0.01%	0.002%
28	6.157	1495	1498	1502	rBV3	645	691	0.01%	0.003%
29	6.250	1512	1527	1548	rBV	407238	773095	16.57%	3.674%
30	6.517	1598	1610	1624	rBV5	13606	30115	0.65%	0.143%
31	6.690	1648	1664	1680	rBV	395227	768204	16.47%	3.651%
32	6.919	1729	1735	1736	rBV2	800	563	0.01%	0.003%
33	6.931	1736	1739	1747	rVB3	822	1044	0.02%	0.005%
34	6.996	1747	1759	1773	rBV2	13487	26400	0.57%	0.125%
35	7.147	1801	1806	1809	rBV2	605	624	0.01%	0.003%
36	7.192	1809	1820	1824	rBV6	3377	5788	0.12%	0.028%

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Integrator: RTE

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Stop Thrs : 0

Peak Location: TOP

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

37	7.298	1849	1853	1856	rBV4	918	796	0.02%	0.004%
38	7.343	1862	1867	1874	rVB4	1874	2545	0.05%	0.012%
39	7.491	1900	1913	1925	rVV	193302	350293	7.51%	1.665%
40	7.565	1925	1936	1958	rVB	222776	394919	8.47%	1.877%
41	7.800	1998	2009	2015	rBV6	4331	8108	0.17%	0.039%
42	7.896	2025	2039	2052	rBV	796592	1380823	29.60%	6.562%
43	7.976	2053	2064	2080	rVB3	278170	602934	12.92%	2.865%
44	8.179	2115	2127	2143	rBV	156216	265103	5.68%	1.260%
45	8.359	2171	2183	2200	rBV	103045	186010	3.99%	0.884%
46	8.574	2236	2250	2259	rBV	89158	154272	3.31%	0.733%
47	8.639	2259	2270	2303	rVV	619966	1117462	23.95%	5.311%
48	8.777	2306	2313	2332	rVB4	13429	26000	0.56%	0.124%
49	8.902	2347	2352	2353	rBV2	782	681	0.01%	0.003%
50	9.018	2376	2388	2406	rVB2	44540	79608	1.71%	0.378%
51	9.169	2427	2435	2448	rVB5	3546	7155	0.15%	0.034%
52	9.246	2452	2459	2462	rBV3	1080	1147	0.02%	0.005%
53	9.275	2465	2468	2475	rVB4	333	367	0.01%	0.002%
54	9.362	2487	2495	2500	rBV5	5261	7272	0.16%	0.035%
55	9.420	2500	2513	2514	rBV	630020	770423	16.52%	3.661%
56	9.632	2573	2579	2580	rBV3	2064	1990	0.04%	0.009%
57	9.783	2623	2626	2630	rBV2	556	413	0.01%	0.002%
58	9.832	2634	2641	2650	rBV5	3339	5656	0.12%	0.027%
59	10.102	2715	2725	2737	rVV3	8104	13968	0.30%	0.066%
60	10.224	2757	2763	2769	rBV6	863	1238	0.03%	0.006%
61	10.481	2837	2843	2845	rBV2	1440	1445	0.03%	0.007%
62	10.652	2886	2896	2909	rBV4	20155	35775	0.77%	0.170%
63	10.758	2915	2929	2949	rBV	641574	1035056	22.19%	4.919%
64	10.851	2954	2958	2964	rVB7	1680	1863	0.04%	0.009%
65	10.896	2969	2972	2977	rVV5	1869	1691	0.04%	0.008%
66	10.928	2977	2982	2987	rVV6	1461	1567	0.03%	0.007%
67	10.983	2988	2999	3011	rVB2	22615	44228	0.95%	0.210%
68	11.098	3025	3035	3047	rVV2	14154	23192	0.50%	0.110%
69	11.195	3062	3065	3066	rBV2	695	398	0.01%	0.002%
70	11.250	3072	3082	3090	rBV5	5452	8638	0.19%	0.041%
71	11.291	3093	3095	3104	rVB4	2411	2526	0.05%	0.012%
72	11.375	3115	3121	3130	rVV3	3052	3808	0.08%	0.018%
73	11.465	3136	3149	3157	rBV7	4654	8333	0.18%	0.040%
74	11.510	3157	3163	3173	rVB5	4248	6533	0.14%	0.031%
75	11.587	3176	3187	3196	rBV4	6593	10878	0.23%	0.052%
76	11.700	3216	3222	3226	rVB6	1097	1296	0.03%	0.006%

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Integration Parameters: LSCINT.P

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

77	11.748	3231	3237	3245	rVB7	3261	4719	0.10%	0.022%
78	11.812	3245	3257	3271	rBV	613147	970944	20.81%	4.614%
79	11.880	3271	3278	3292	rVB6	19549	35608	0.76%	0.169%
80	11.951	3293	3300	3303	rBV7	1799	2461	0.05%	0.012%
81	12.195	3361	3376	3397	rVV	792313	1394497	29.89%	6.627%
82	12.394	3435	3438	3446	rVB5	1003	1299	0.03%	0.006%
83	12.475	3456	3463	3468	rBV7	1226	1540	0.03%	0.007%
84	12.684	3523	3528	3531	rBV4	1372	1476	0.03%	0.007%
85	12.770	3549	3555	3562	rBV3	2260	3067	0.07%	0.015%
86	12.973	3605	3618	3626	rVB8	2546	5038	0.11%	0.024%
87	13.034	3630	3637	3641	rVB3	674	1000	0.02%	0.005%
88	13.330	3725	3729	3733	rBV3	511	451	0.01%	0.002%
89	13.375	3733	3743	3753	rVV3	19887	29698	0.64%	0.141%
90	13.452	3764	3767	3774	rVB5	1227	1136	0.02%	0.005%
91	13.735	3851	3855	3858	rBV3	976	905	0.02%	0.004%
92	13.777	3864	3868	3869	rBV3	1096	849	0.02%	0.004%
93	13.844	3885	3889	3894	rBV2	695	829	0.02%	0.004%
94	14.092	3962	3966	3974	rVB3	1872	2340	0.05%	0.011%
95	14.333	4038	4041	4046	rVB2	758	703	0.02%	0.003%
96	14.365	4046	4051	4058	rBV4	783	997	0.02%	0.005%
97	14.430	4065	4071	4079	rVB6	5181	6288	0.13%	0.030%
98	14.494	4080	4091	4111	rVV2	99908	171053	3.67%	0.813%
99	15.545	4408	4418	4429	rVB2	42721	66262	1.42%	0.315%
100	16.391	4674	4681	4690	rBV5	9816	13753	0.29%	0.065%

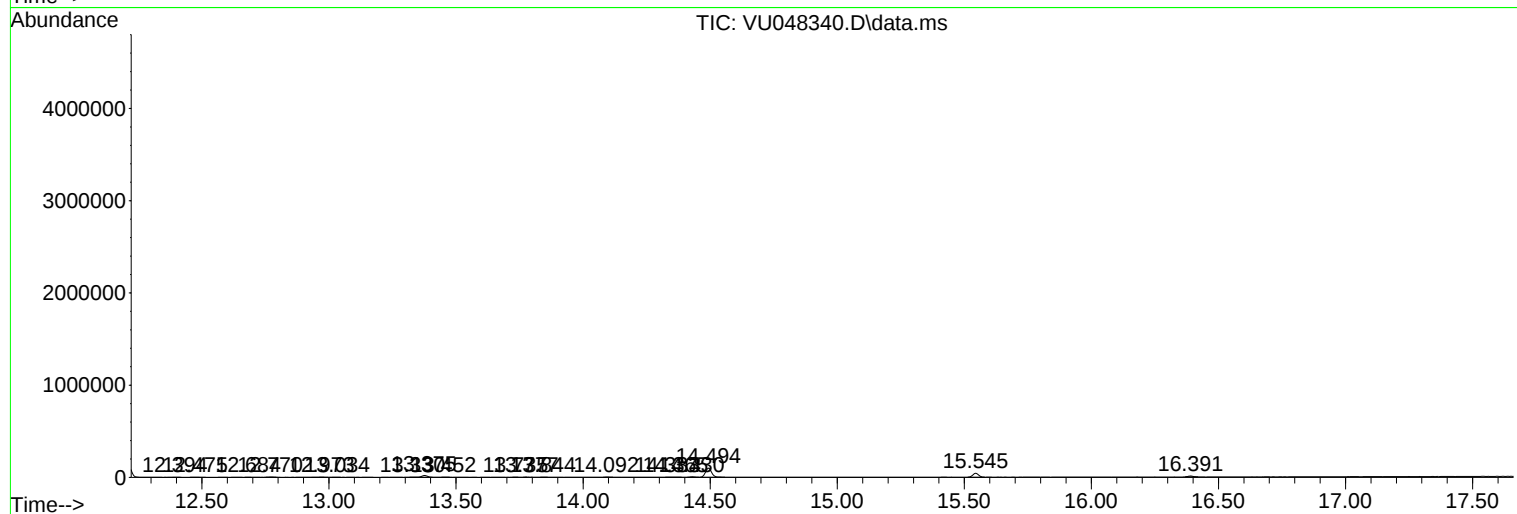
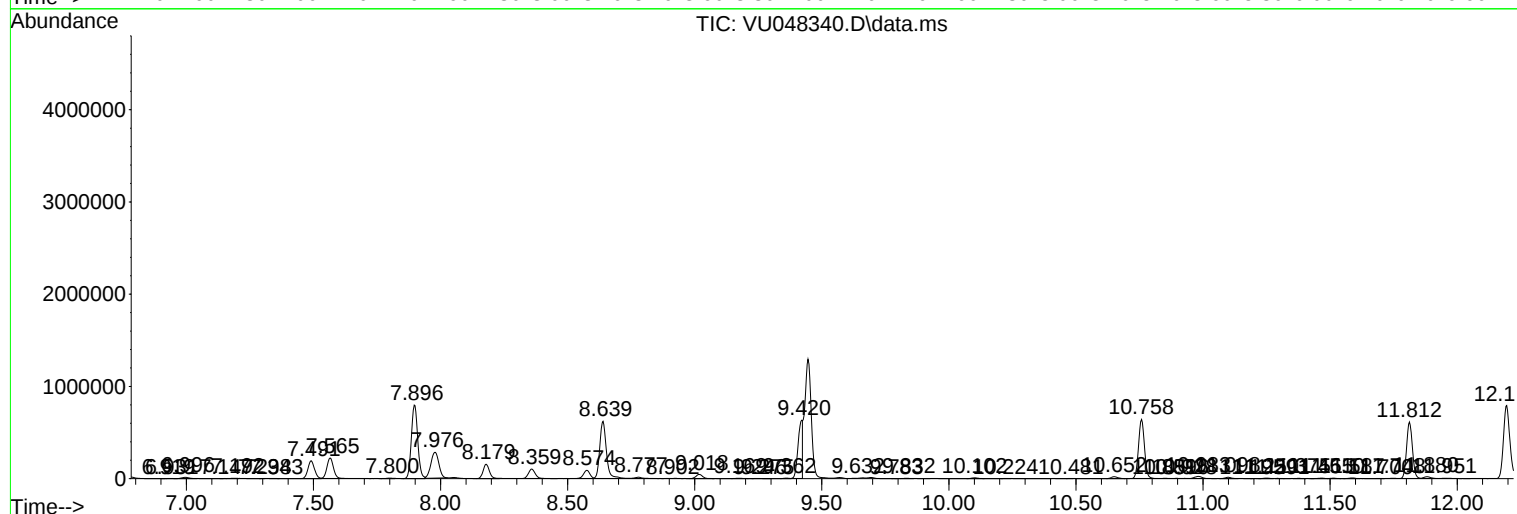
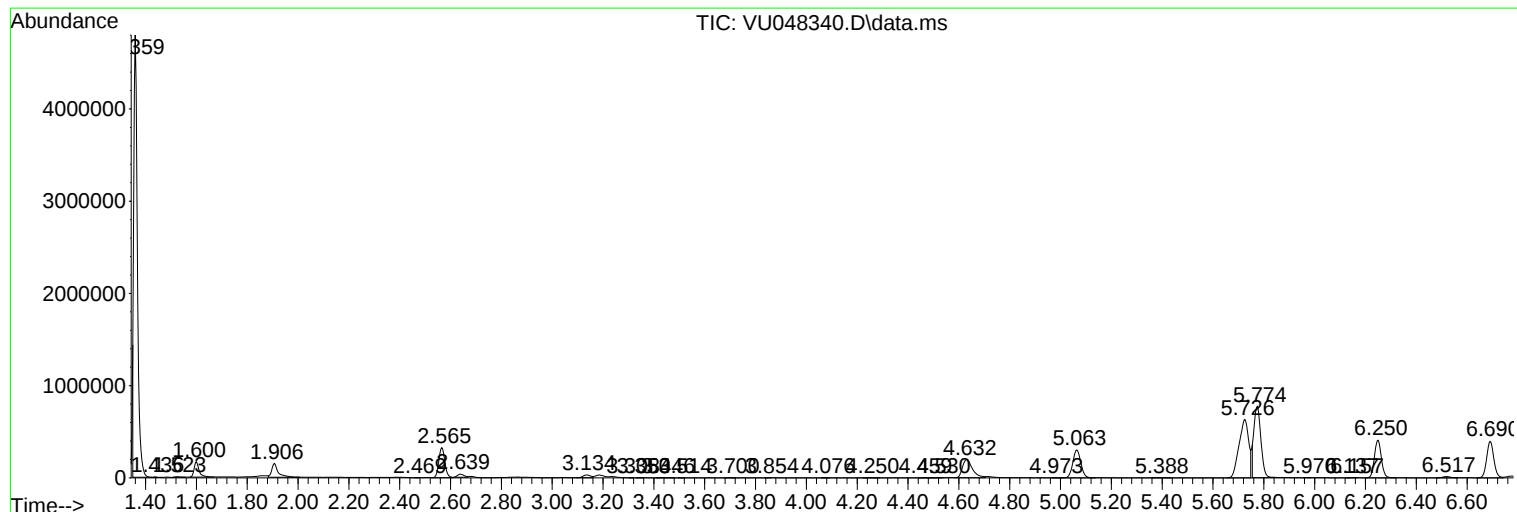
Sum of corrected areas: 21042013

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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXET6DL

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\VU042822\
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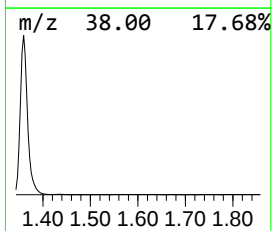
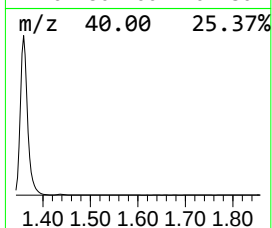
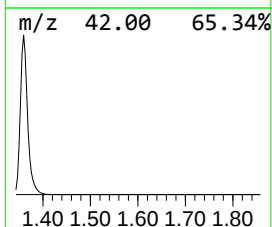
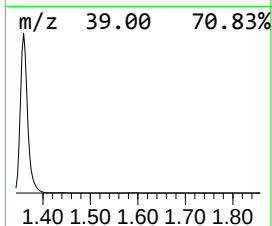
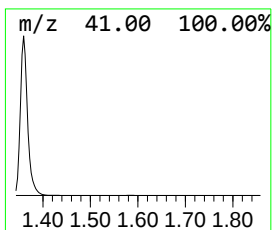
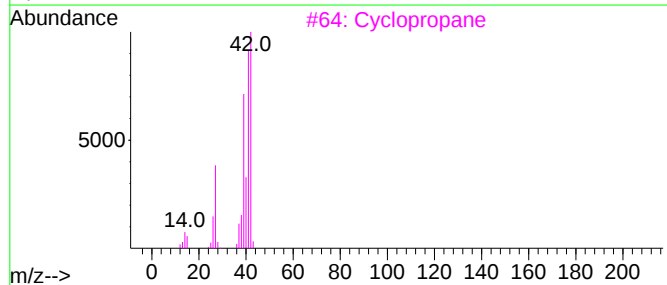
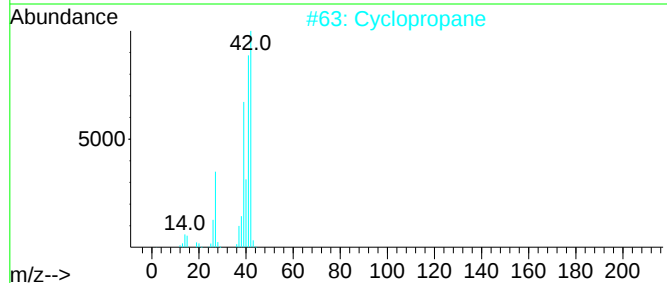
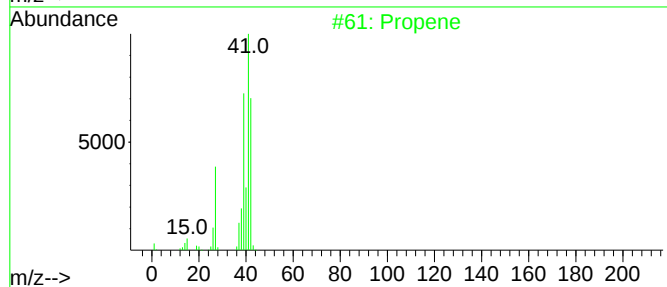
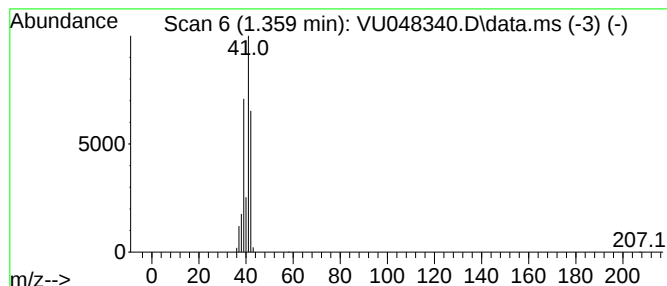
Instrument :
MSVOA_U
ClientSampleId :
EXET6DL

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 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.359	301.70 ug/L	4664920	1,4-Difluorobenzene	6.250	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	90
2	Cyclopropane	42	C3H6	000075-19-4	78
3	Cyclopropane	42	C3H6	000075-19-4	78
4	Propene	42	C3H6	000115-07-1	50
5	Cyclopropene	40	C3H4	002781-85-3	16



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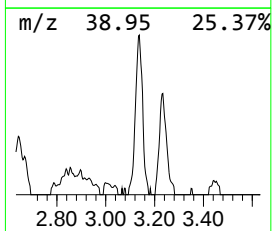
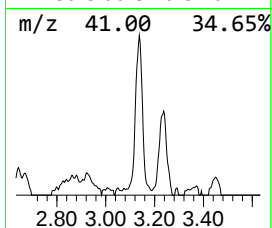
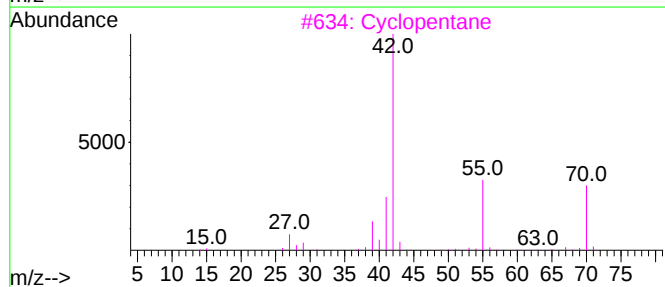
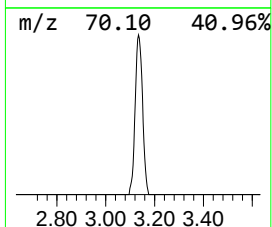
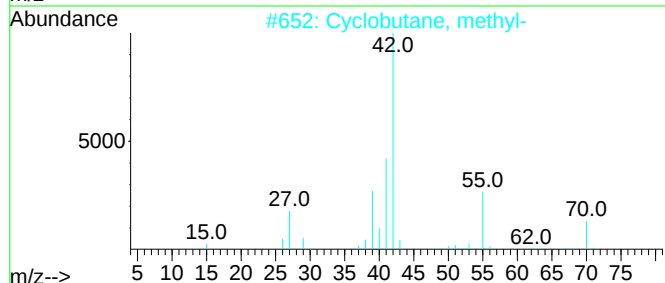
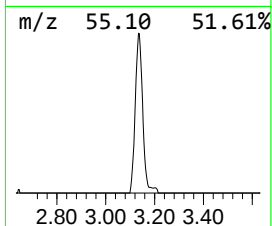
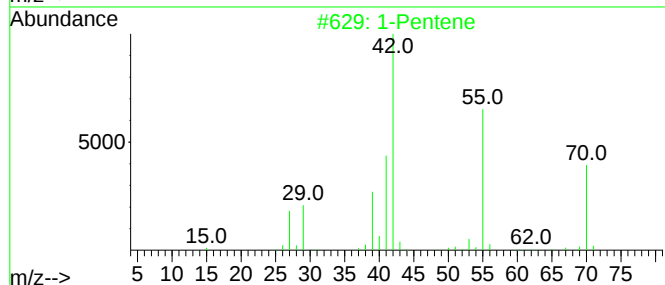
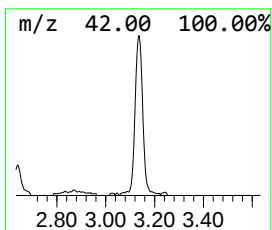
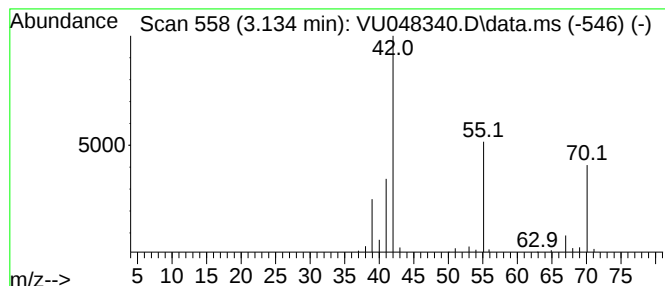
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.134	3.99 ug/L	61650	1,4-Difluorobenzene	6.250

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Pentene	70	C5H10	000109-67-1	87
2		Cyclobutane, methyl-	70	C5H10	000598-61-8	86
3		Cyclopentane	70	C5H10	000287-92-3	86
4		Cyclopropane, ethyl-	70	C5H10	001191-96-4	86
5		Cyclopentane	70	C5H10	000287-92-3	83



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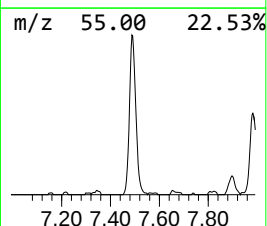
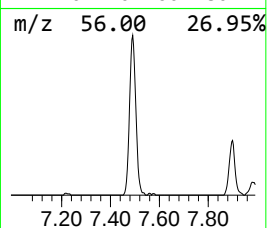
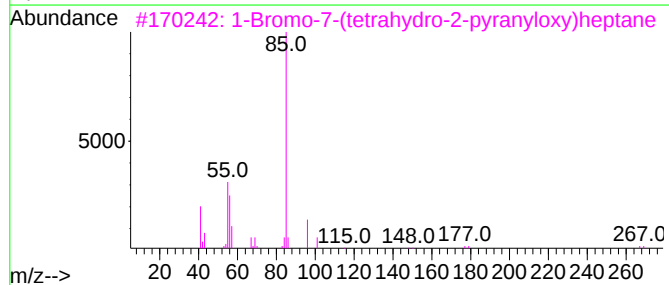
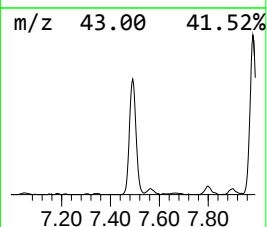
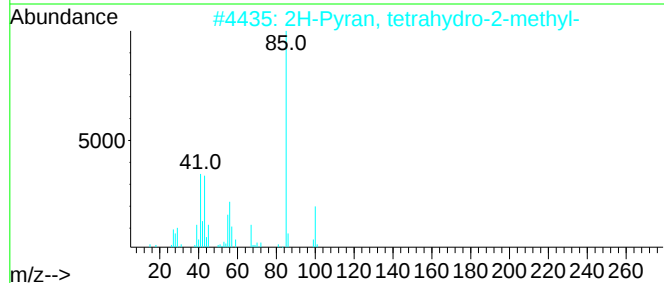
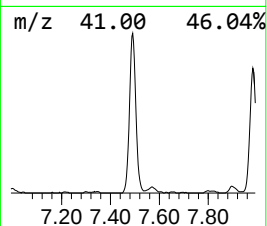
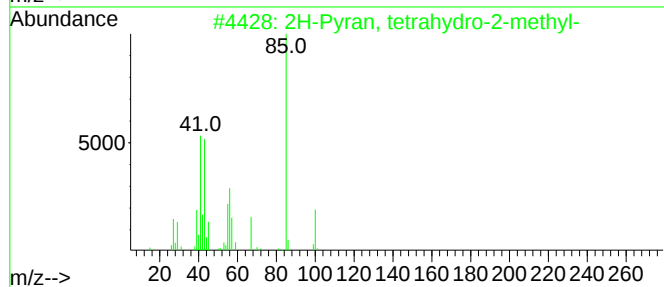
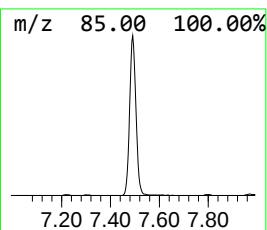
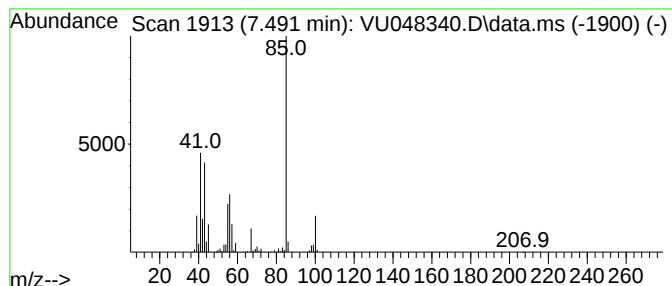
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 2H-Pyran, tetrahydro-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.491	22.66 ug/L	350293	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Pyran, tetrahydro-2-methyl-			100	C6H12O	010141-72-7	97
2	2H-Pyran, tetrahydro-2-methyl-			100	C6H12O	010141-72-7	86
3	1-Bromo-7-(tetrahydro-2-pyranyloxy)heptane			278	C12H23BrO2	010160-25-5	59
4	2H-Pyran, tetrahydro-2-methyl-			100	C6H12O	010141-72-7	59
5	Oxetane, 2-ethyl-3-methyl-			100	C6H12O	053778-62-4	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042822\
Data File : VU048340.D
Acq On : 28 Apr 2022 14:50
Operator : SY/MD
Sample : N2587-10DL 40X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXET6DL

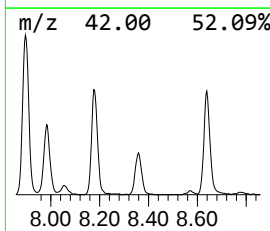
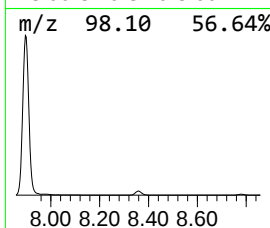
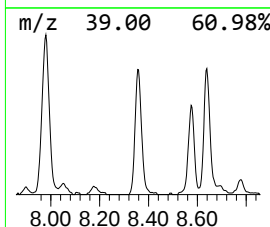
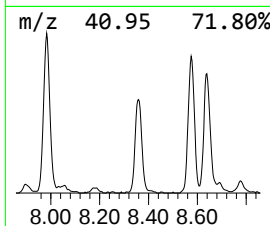
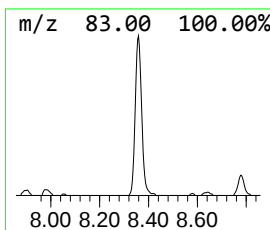
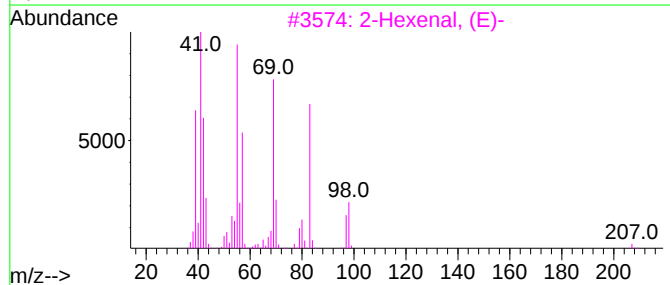
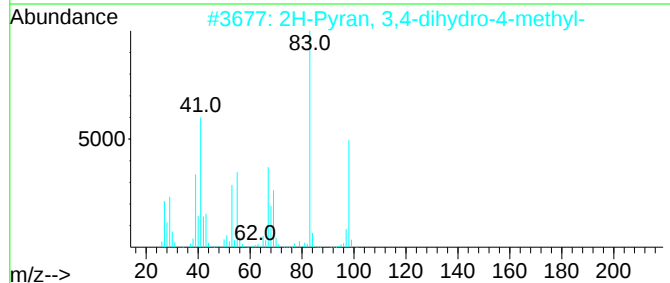
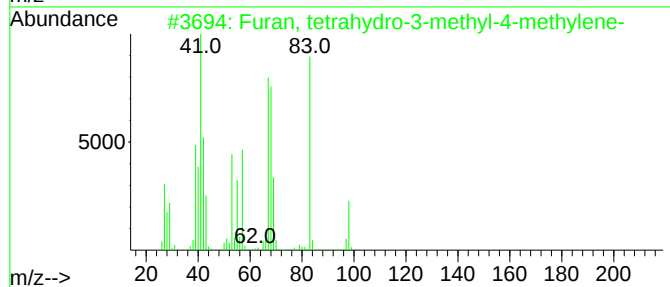
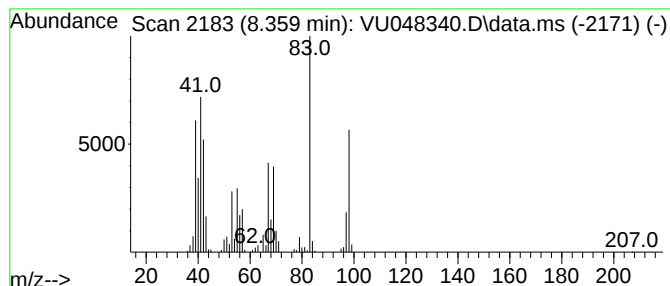
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Quant Title : VOC Analysis

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

Peak Number 5 Furan, tetrahydro-3-methyl-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.359	12.07 ug/L	186010	Chlorobenzene-d5	9.417

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, tetrahydro-3-methyl-4-met...	98	C6H10O	061142-01-6	76
2	2H-Pyran, 3,4-dihydro-4-methyl-	98	C6H10O	002270-61-3	70
3	2-Hexenal, (E)-	98	C6H10O	006728-26-3	53
4	4,4-Dimethyl-2-imidazoline	98	C5H10N2	002305-59-1	49
5	1H-Pyrazole, 4,5-dihydro-4,5-dim...	98	C5H10N2	028019-94-5	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042822\
Data File : VU048340.D
Acq On : 28 Apr 2022 14:50
Operator : SY/MD
Sample : N2587-10DL 40X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXET6DL

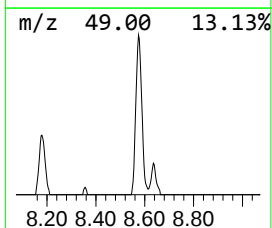
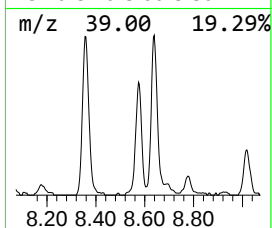
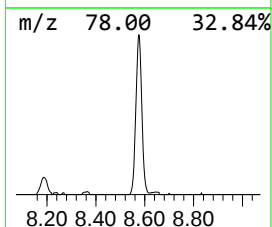
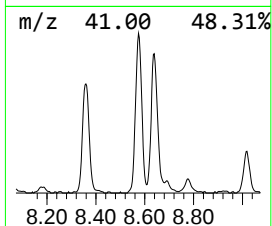
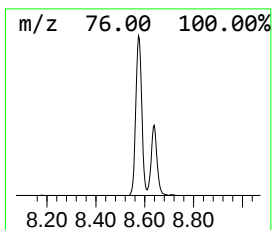
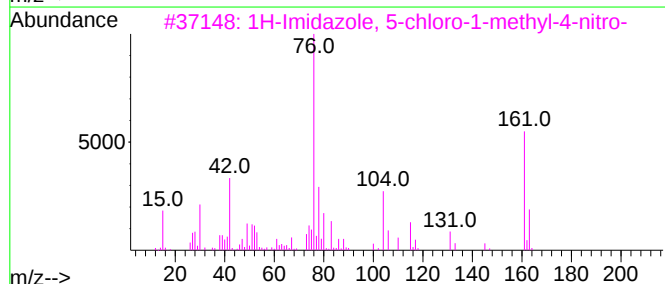
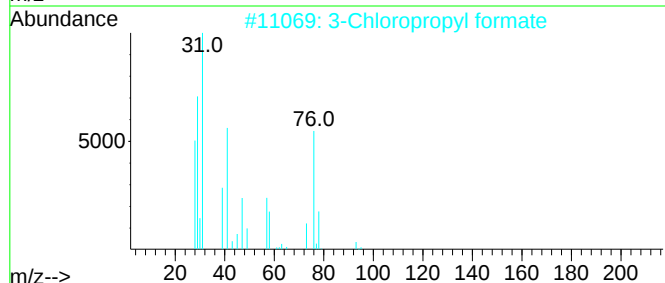
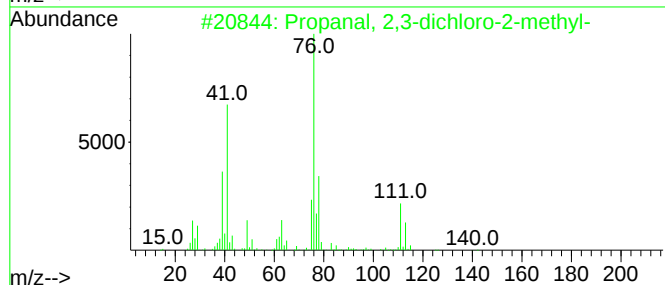
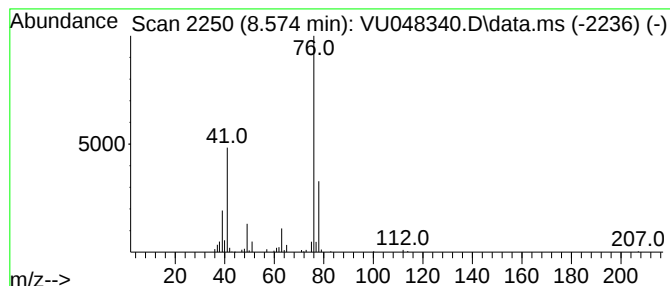
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Quant Title : VOC Analysis

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

Peak Number 6 Propanal, 2,3-dichloro-2-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.574	10.01 ug/L	154272	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal, 2,3-dichloro-2-methyl-	140	C4H6Cl2O	010141-22-7	64
2			3-Chloropropyl formate	122	C4H7ClO2	001487-44-1	43
3			1H-Imidazole, 5-chloro-1-methyl-...	161	C4H4ClN3O2	004897-25-0	43
4			Propane, 1,3-dichloro-	112	C3H6Cl2	000142-28-9	15
5			Propane, 1,3-dichloro-	112	C3H6Cl2	000142-28-9	15



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042822\
Data File : VU048340.D
Acq On : 28 Apr 2022 14:50
Operator : SY/MD
Sample : N2587-10DL 40X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXET6DL

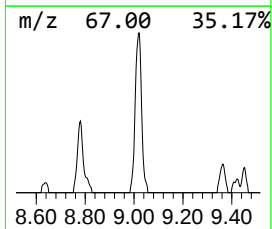
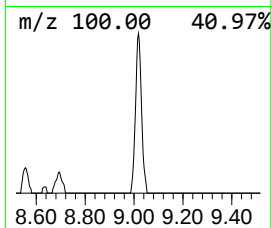
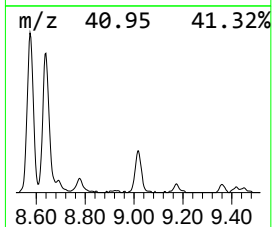
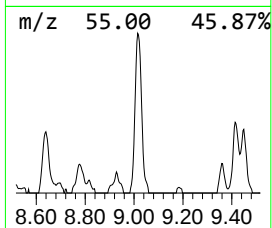
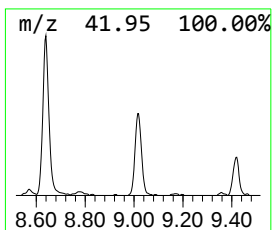
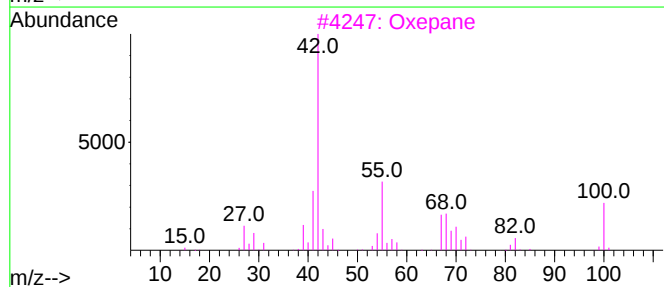
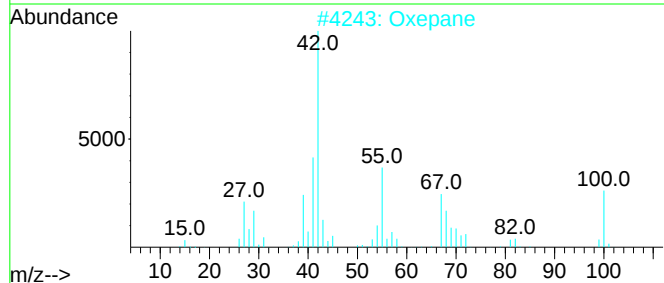
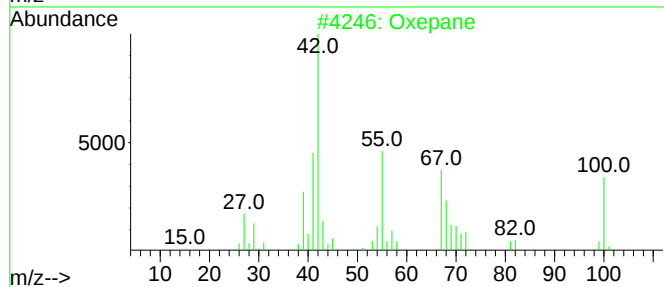
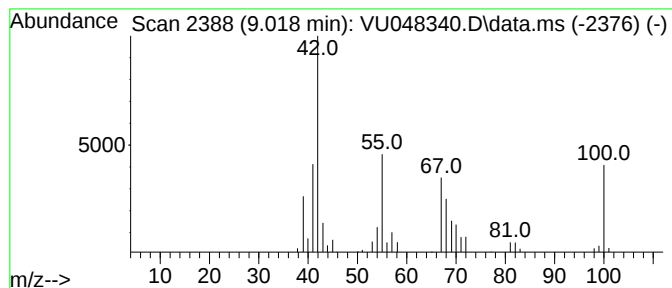
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Quant Title : VOC Analysis

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

Peak Number 7 Oxepane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.018	5.17 ug/L	79608	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxepane			100	C6H12O	000592-90-5	96
2	Oxepane			100	C6H12O	000592-90-5	95
3	Oxepane			100	C6H12O	000592-90-5	83
4	Oxepane			100	C6H12O	000592-90-5	59
5	3(2H)-Furanone, dihydro-5-methyl-			100	C5H8O2	034003-72-0	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042822\
Data File : VU048340.D
Acq On : 28 Apr 2022 14:50
Operator : SY/MD
Sample : N2587-10DL 40X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXET6DL

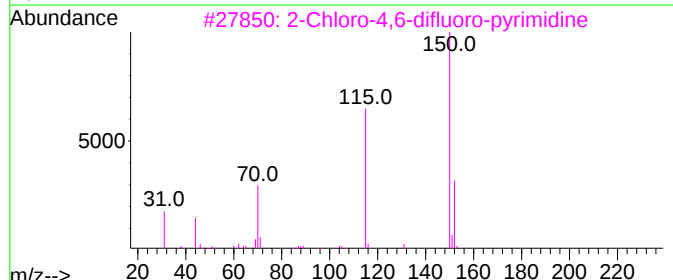
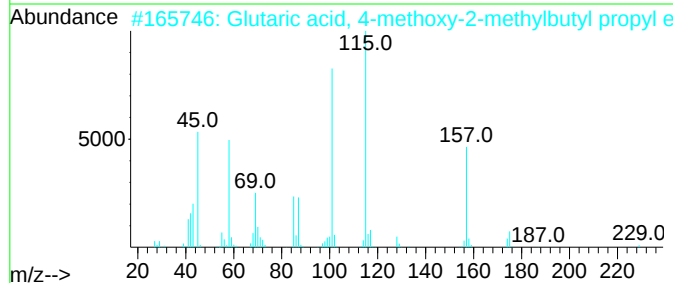
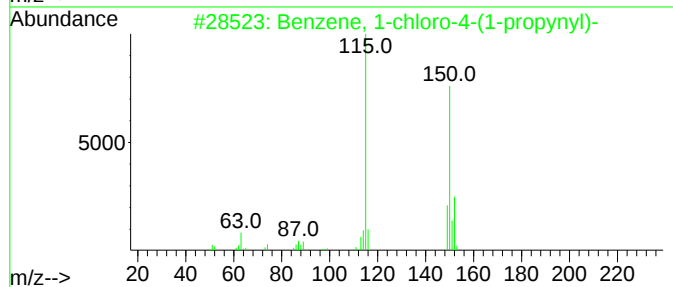
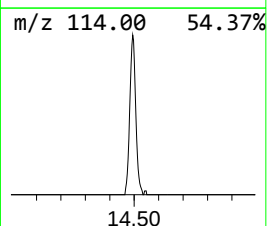
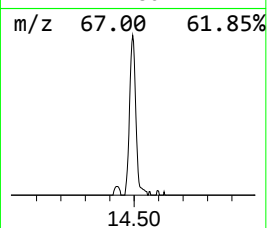
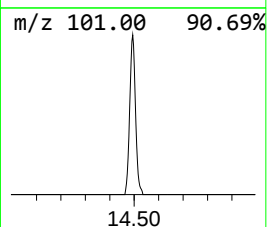
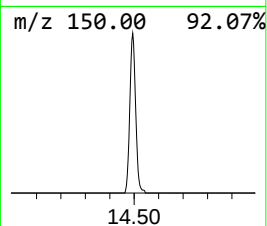
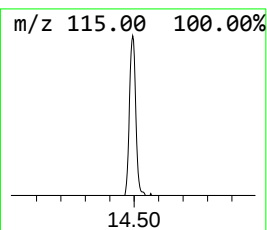
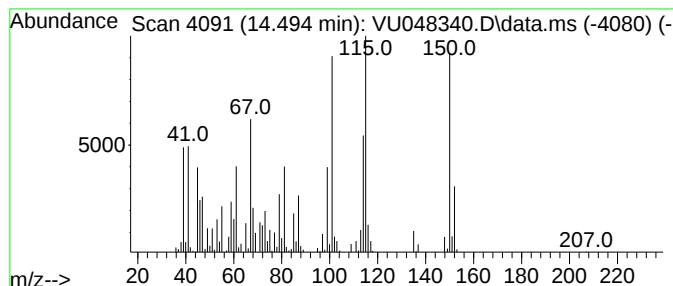
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Quant Title : VOC Analysis

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

Peak Number 8 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.494	8.81 ug/L	171053	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-chloro-4-(1-propynyl)-	150	C9H7Cl	002809-65-6	38
2			Glutaric acid, 4-methoxy-2-methylbutyl propyl ester	274	C14H26O5	1010359-41-0	27
3			2-Chloro-4,6-difluoro-pyrimidine	150	C4HClF2N2	038953-30-9	18
4			Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	15
5			2-Pyrrolidinethione, 1-methyl-	115	C5H9NS	010441-57-3	11



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042822\
Data File : VU048340.D
Acq On : 28 Apr 2022 14:50
Operator : SY/MD
Sample : N2587-10DL 40X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXET6DL

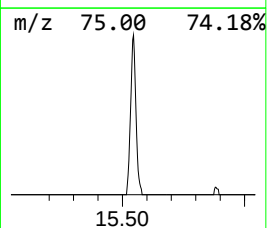
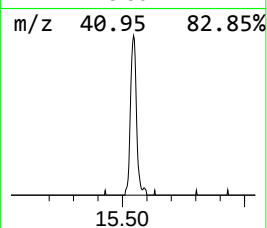
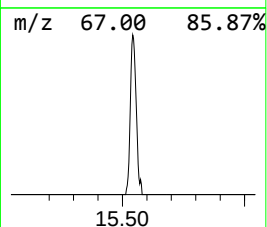
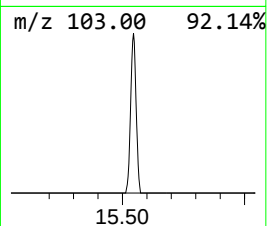
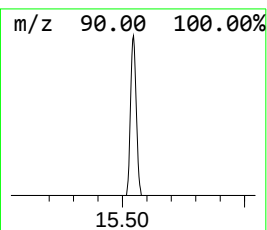
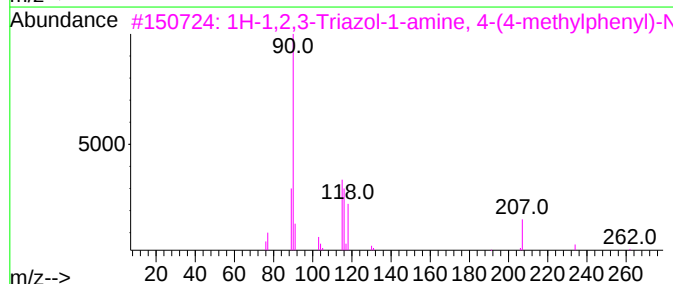
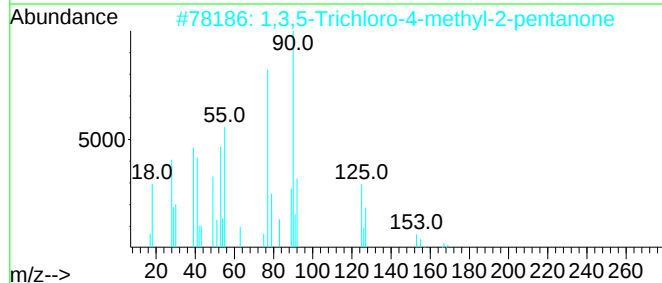
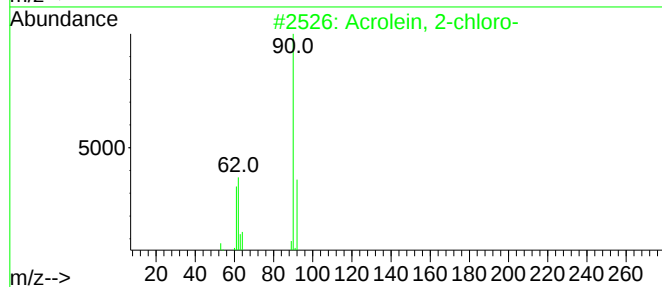
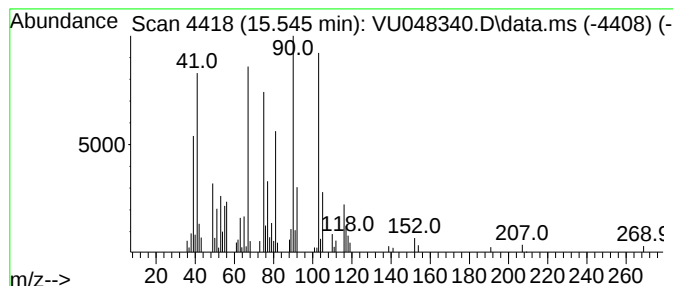
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

Peak Number 9 unknown-02 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.545	3.41 ug/L	66262	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acrolein, 2-chloro-	90	C3H3ClO	000683-51-2	38
2			1,3,5-Trichloro-4-methyl-2-penta...	202	C6H9Cl3O	1000140-03-8	37
3			1H-1,2,3-Triazol-1-amine, 4-(4-m...	262	C16H14N4	113261-43-1	36
4			Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	25
5			2,2-Bis(chloromethyl)-1-propanol	156	C5H10Cl2O	005355-54-4	23



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042822\
Data File : VU048340.D
Acq On : 28 Apr 2022 14:50
Operator : SY/MD
Sample : N2587-10DL 40X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXET6DL

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	1.359	301.7	ug/L	4664920	1	6.250	773095	50.0
(DEL) Alkane: S...	3.134	4.0	ug/L	61650	1	6.250	773095	50.0
2H-Pyran, tetra...	7.491	22.7	ug/L	350293	1	6.250	773095	50.0
Furan, tetrahyd...	8.359	12.1	ug/L	186010	2	9.417	770423	50.0
Propanal, 2,3-d...	8.574	10.0	ug/L	154272	2	9.417	770423	50.0
Oxepane	9.018	5.2	ug/L	79608	2	9.417	770423	50.0
unknown-01	14.494	8.8	ug/L	171053	3	11.812	970944	50.0
unknown-02	15.545	3.4	ug/L	66262	3	11.812	970944	50.0