

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062723\
 Data File : VX036343.D
 Acq On : 27 Jun 2023 11:59
 Operator : JC/MD
 Sample : VX0627MBL01
 Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VX0627MBL01

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % 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_X\Method\82X062323W.M
 Title : SW846 8260

Signal : TIC: VX036343.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	7	9	17	rVB2	4200	5209	20.18%	1.477%
2	1.215	17	21	24	rVB2	404	581	2.25%	0.165%
3	1.264	26	29	31	rBV3	1538	1661	6.43%	0.471%
4	1.294	31	34	35	rBV3	1086	1376	5.33%	0.390%
5	1.374	45	47	53	rVB7	1506	2289	8.87%	0.649%
6	2.319	199	202	205	rVB3	1123	1464	5.67%	0.415%
7	2.398	210	215	216	rBV4	919	1304	5.05%	0.370%
8	2.514	230	234	240	rVB2	2727	4719	18.28%	1.338%
9	2.794	274	280	287	rVB4	1813	4055	15.71%	1.150%
10	3.087	320	328	339	rBV7	2198	6398	24.78%	1.815%
11	3.440	383	386	389	rBV	530	741	2.87%	0.210%
12	3.568	405	407	409	rVB2	389	402	1.56%	0.114%
13	3.599	409	412	413	rBV2	353	420	1.63%	0.119%
14	3.727	427	433	436	rBV2	1126	2192	8.49%	0.622%
15	4.013	479	480	484	rBV	326	388	1.50%	0.110%
16	4.465	552	554	556	rBV2	666	730	2.83%	0.207%
17	4.580	563	573	586	rBV	4682	17669	68.43%	5.011%
18	4.861	614	619	620	rBV	455	506	1.96%	0.144%
19	5.025	644	646	648	rBV2	544	637	2.47%	0.181%
20	5.068	652	653	656	rBV2	509	438	1.70%	0.124%
21	5.373	696	703	704	rBV	3777	4913	19.03%	1.393%
22	5.550	722	732	739	rBV3	7945	19186	74.31%	5.442%
23	5.696	754	756	759	rVB3	514	455	1.76%	0.129%
24	5.952	791	798	807	rBV4	3547	9513	36.84%	2.698%
25	6.763	924	931	941	rVB2	10605	25819	100.00%	7.323%
26	6.854	941	946	947	rBV2	337	486	1.88%	0.138%
27	6.909	953	955	961	rVB3	262	406	1.57%	0.115%
28	7.116	984	989	990	rBV3	704	940	3.64%	0.267%
29	7.373	1026	1031	1034	rBV3	523	569	2.20%	0.161%
30	7.580	1061	1065	1066	rBV3	631	904	3.50%	0.256%
31	7.702	1082	1085	1090	rVB3	406	500	1.94%	0.142%
32	7.830	1104	1106	1110	rVB	574	458	1.77%	0.130%
33	7.958	1126	1127	1132	rBV2	368	413	1.60%	0.117%
34	8.110	1148	1152	1153	rBV2	271	406	1.57%	0.115%
35	8.238	1168	1173	1183	rVB3	1348	2620	10.15%	0.743%
36	8.372	1190	1195	1197	rBV2	703	764	2.96%	0.217%

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Integrator: RTE

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37	8.452	1203	1208	1210	rBV2	337	523	2.03%	0.148%
38	8.574	1222	1228	1233	rBV3	2205	2863	11.09%	0.812%
39	8.647	1234	1240	1247	rVV	14948	23477	90.93%	6.659%
40	8.714	1247	1251	1256	rVB2	862	1496	5.79%	0.424%
41	8.976	1291	1294	1300	rVB2	1048	1748	6.77%	0.496%
42	9.116	1315	1317	1319	rBV	564	559	2.17%	0.159%
43	9.195	1327	1330	1335	rBV2	336	685	2.65%	0.194%
44	9.275	1339	1343	1346	rVV3	1656	2366	9.16%	0.671%
45	9.305	1346	1348	1352	rVB3	687	1029	3.99%	0.292%
46	9.433	1364	1369	1377	rVB2	1815	2725	10.55%	0.773%
47	9.518	1380	1383	1386	rBV	500	452	1.75%	0.128%
48	9.579	1390	1393	1396	rVV2	453	584	2.26%	0.166%
49	9.610	1396	1398	1402	rVB	481	549	2.13%	0.156%
50	9.695	1408	1412	1420	rVB3	1653	2278	8.82%	0.646%
51	10.055	1466	1471	1479	rVB2	10695	16377	63.43%	4.645%
52	10.195	1491	1494	1496	rVB	1416	1354	5.24%	0.384%
53	10.299	1507	1511	1518	rVB	3651	4997	19.35%	1.417%
54	10.646	1562	1568	1573	rBV5	2529	4060	15.72%	1.152%
55	10.799	1591	1593	1596	rVB3	423	414	1.60%	0.117%
56	10.841	1596	1600	1604	rBV3	1162	1394	5.40%	0.395%
57	10.963	1616	1620	1626	rVV3	2046	2713	10.51%	0.769%
58	11.018	1626	1629	1634	rVV3	876	998	3.87%	0.283%
59	11.079	1635	1639	1647	rVB3	6510	8700	33.70%	2.468%
60	11.195	1654	1658	1662	rBV3	1628	2701	10.46%	0.766%
61	11.299	1672	1675	1681	rVV	3082	3929	15.22%	1.114%
62	11.366	1681	1686	1691	rVB4	2141	3590	13.90%	1.018%
63	11.451	1696	1700	1708	rVB2	5506	7108	27.53%	2.016%
64	11.713	1739	1743	1747	rBV2	3169	4338	16.80%	1.230%
65	11.750	1747	1749	1755	rVB2	3112	3159	12.24%	0.896%
66	11.890	1768	1772	1776	rBV4	4376	5263	20.38%	1.493%
67	11.969	1780	1785	1788	rBV2	3744	4693	18.18%	1.331%
68	12.018	1788	1793	1800	rVV5	7685	18776	72.72%	5.325%
69	12.213	1821	1825	1828	rVB3	736	1232	4.77%	0.349%
70	12.329	1840	1844	1852	rVB3	8641	11029	42.72%	3.128%
71	12.536	1875	1878	1885	rVB3	1484	1906	7.38%	0.541%
72	12.853	1925	1930	1934	rVB4	672	993	3.85%	0.282%
73	12.939	1942	1944	1947	rVB3	572	553	2.14%	0.157%
74	13.182	1980	1984	1987	rBV3	294	565	2.19%	0.160%
75	13.286	1993	2001	2005	rBV2	5377	7557	29.27%	2.143%
76	13.512	2035	2038	2041	rVB2	397	422	1.63%	0.120%

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 ClientSampleId :
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Integrator: RTE

Smoothing : ON

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 Title : SW846 8260

77	13.585	2044	2050	2056	rVV3	7108	9692	37.54%	2.749%
78	13.682	2061	2066	2069	rVV5	923	1595	6.18%	0.452%
79	13.719	2069	2072	2077	rVV2	10832	13684	53.00%	3.881%
80	13.774	2077	2081	2090	rVV	9012	12729	49.30%	3.610%
81	13.859	2092	2095	2096	rBV3	570	466	1.80%	0.132%
82	13.957	2107	2111	2119	rVB2	8523	11317	43.83%	3.210%
83	14.030	2119	2123	2125	rBV2	491	752	2.91%	0.213%
84	14.390	2180	2182	2185	rVB2	510	449	1.74%	0.127%
85	14.451	2191	2192	2196	rVB4	791	917	3.55%	0.260%
86	14.676	2225	2229	2231	rBV3	713	877	3.40%	0.249%
87	14.700	2231	2233	2235	rVV2	612	527	2.04%	0.149%
88	14.725	2235	2237	2239	rVV2	643	576	2.23%	0.163%
89	14.780	2241	2246	2248	rBV4	983	1629	6.31%	0.462%
90	14.853	2256	2258	2262	rVB4	426	524	2.03%	0.149%
91	15.103	2297	2299	2301	rBV2	559	530	2.05%	0.150%
92	15.322	2333	2335	2337	rBV2	520	650	2.52%	0.184%
93	15.420	2348	2351	2353	rBV4	569	622	2.41%	0.176%
94	15.536	2366	2370	2376	rBV5	3017	5450	21.11%	1.546%
95	15.621	2383	2384	2385	rBV	747	393	1.52%	0.111%
96	16.468	2519	2523	2528	rBV8	2678	4895	18.96%	1.388%
97	16.596	2542	2544	2546	rVB2	980	644	2.49%	0.183%
98	16.664	2553	2555	2558	rBV2	501	592	2.29%	0.168%
99	16.694	2558	2560	2564	rVV5	574	785	3.04%	0.223%
100	16.755	2569	2570	2571	rBV	951	602	2.33%	0.171%

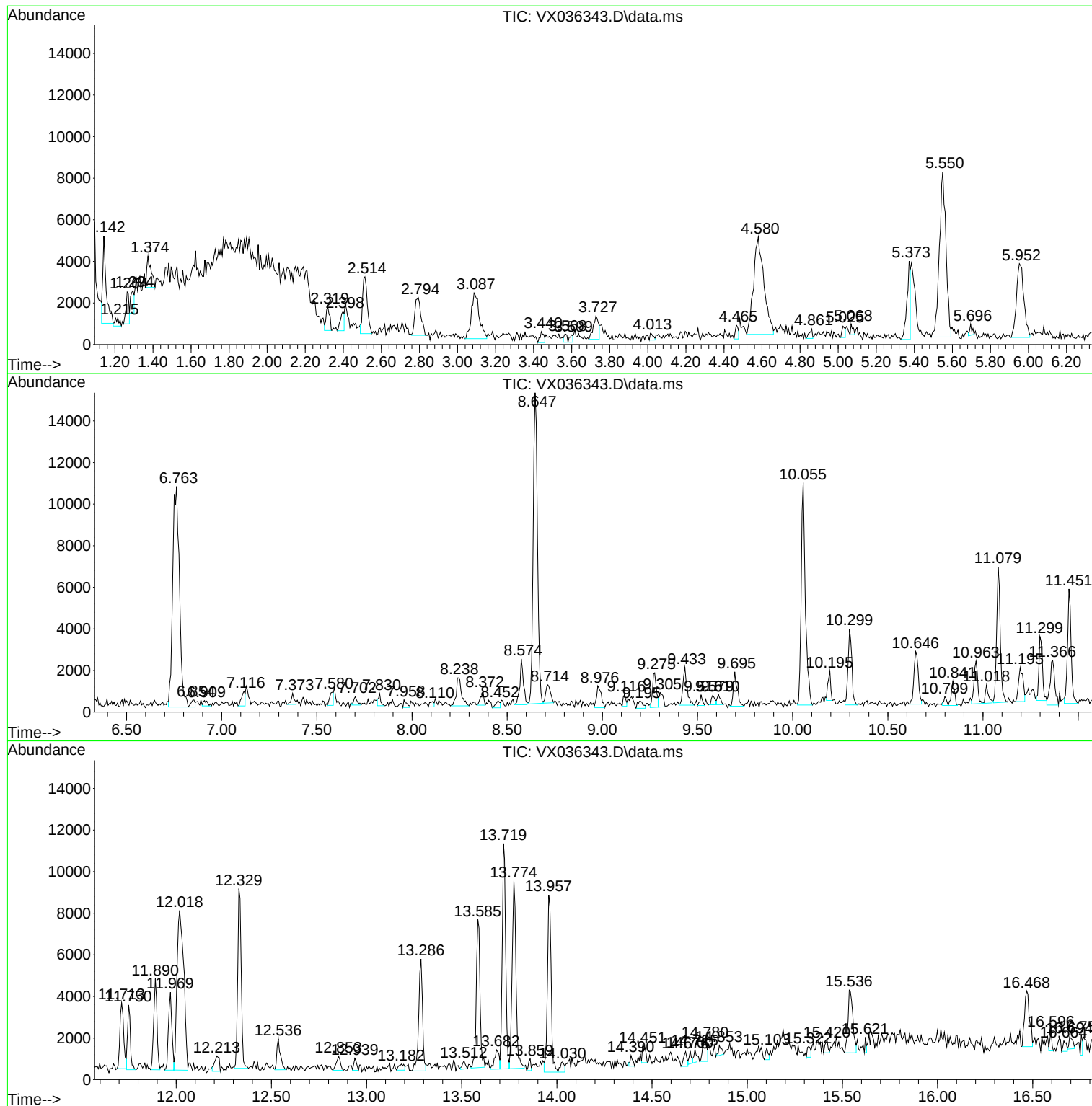
Sum of corrected areas: 352583

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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

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



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MSVOA_X
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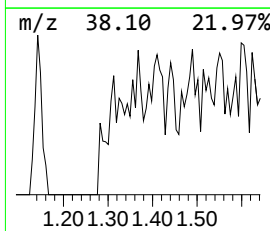
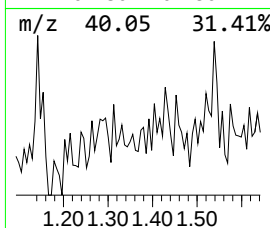
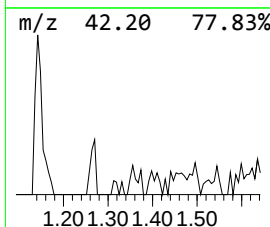
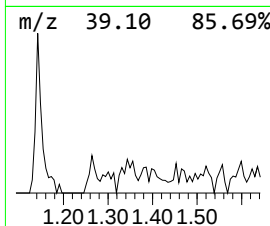
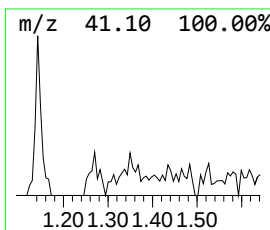
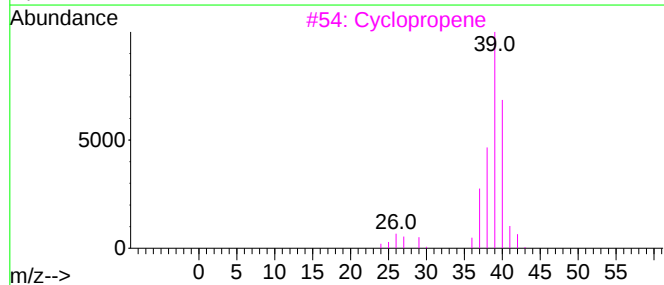
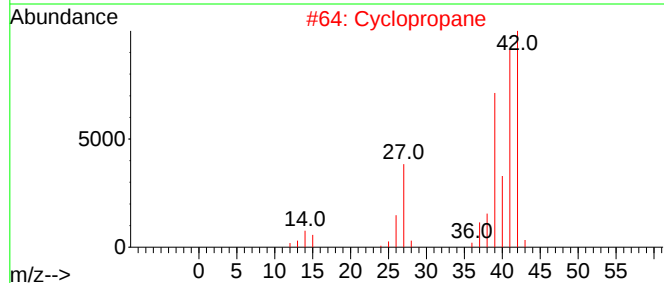
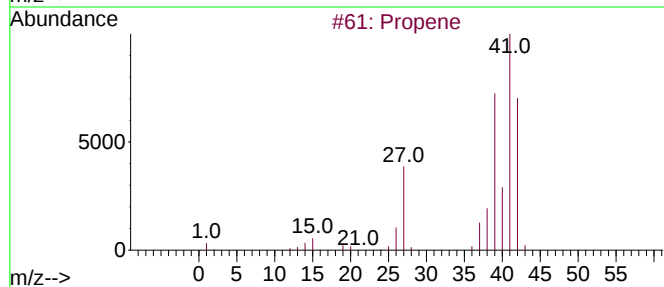
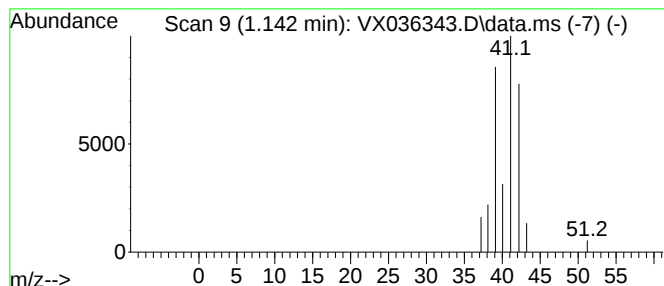
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

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

Peak Number 1 Propene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.142	13.57 ug/l	5209	Pentafluorobenzene	5.544

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	90
2			Cyclopropane	42	C3H6	000075-19-4	72
3			Cyclopropene	40	C3H4	002781-85-3	9
4			2-Oxetanone, 4-methyl-	86	C4H6O2	003068-88-0	4
5			4-Amino-1-butanol	89	C4H11NO	013325-10-5	1



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VX0627MBL01

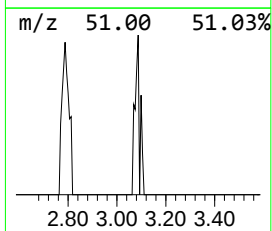
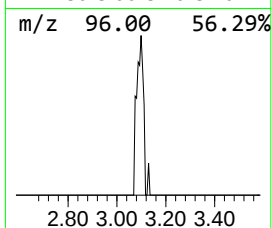
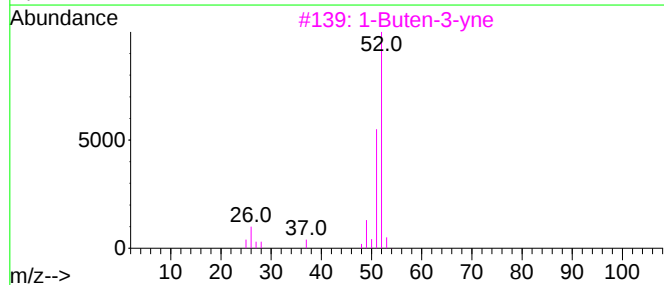
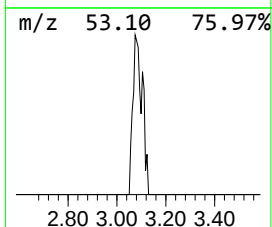
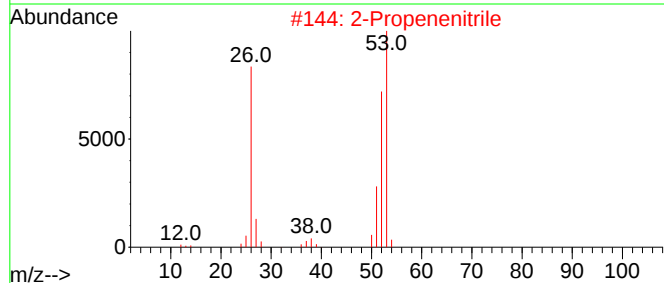
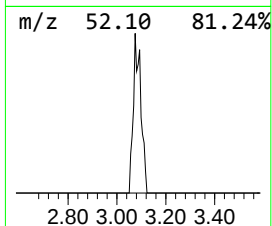
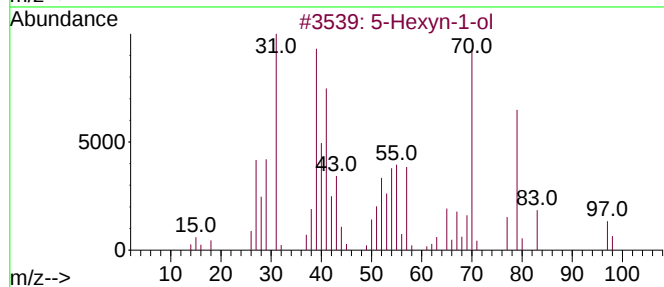
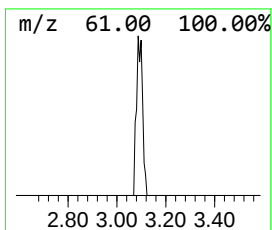
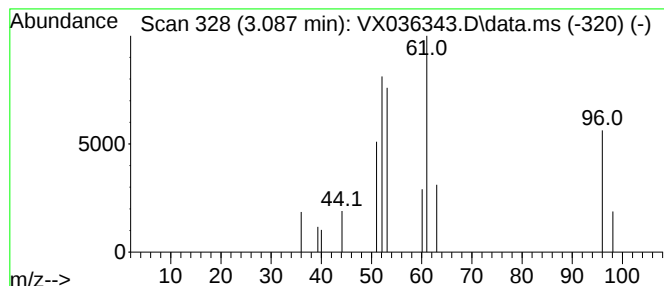
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

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

Peak Number 3 unknown3.087 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.087	16.67 ug/l	6398	Pentafluorobenzene	5.544

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Hexyn-1-ol			98	C6H10O	000928-90-5	39
2	2-Propenenitrile			53	C3H3N	000107-13-1	7
3	1-Buten-3-yne			52	C4H4	000689-97-4	5
4	Cyanogen			52	C2N2	000460-19-5	3
5	Propiolic acid			70	C3H2O2	000471-25-0	2



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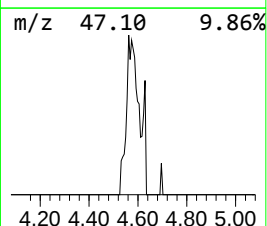
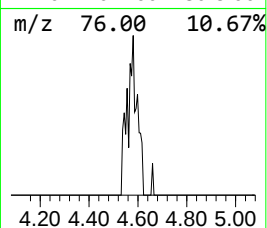
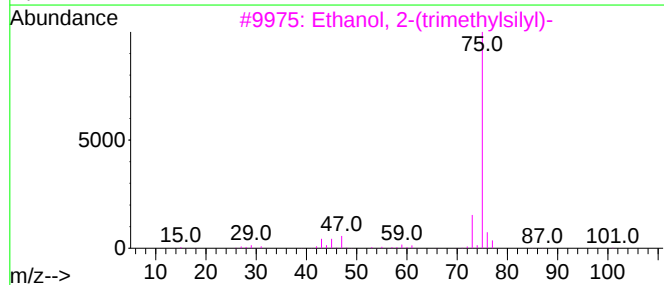
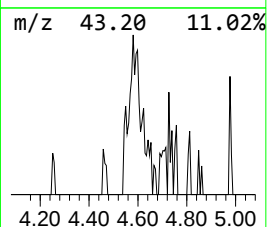
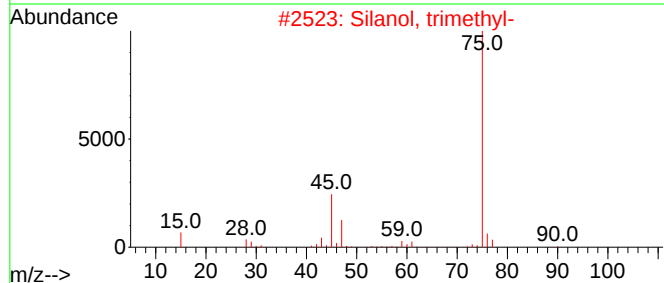
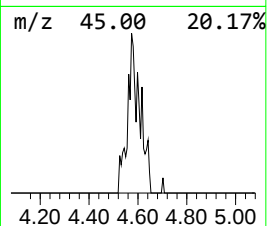
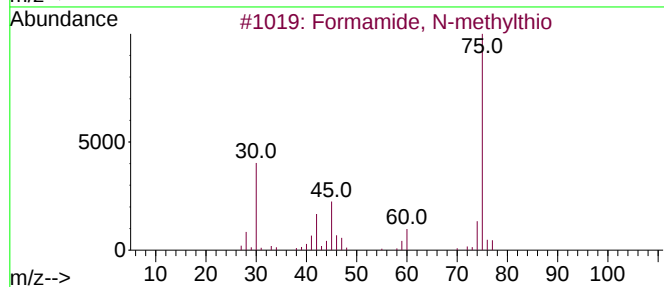
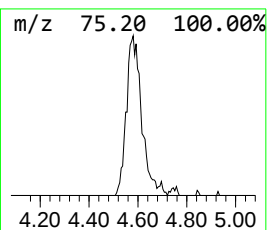
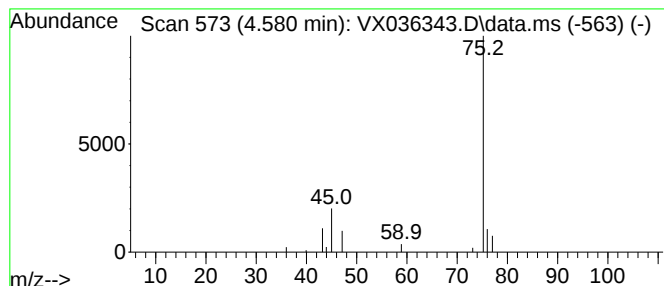
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Quant Title : SW846 8260

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

Peak Number 5 Formamide, N-methylthio Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.580	46.05 ug/l	17669	Pentafluorobenzene	5.544

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Formamide, N-methylthio	75	C2H5NS	018952-41-5	83
2			Silanol, trimethyl-	90	C3H10OSi	001066-40-6	74
3			Ethanol, 2-(trimethylsilyl)-	118	C5H14OSi	002916-68-9	40
4			Ethanethioamide	75	C2H5NS	000062-55-5	7
5			Mercaptamine	77	C2H7NS	000060-23-1	7



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062723\
Data File : VX036343.D
Acq On : 27 Jun 2023 11:59
Operator : JC/MD
Sample : VX0627MBL01
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VX0627MBL01

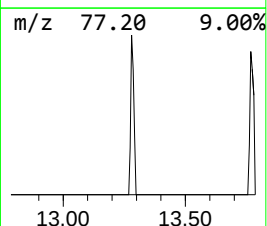
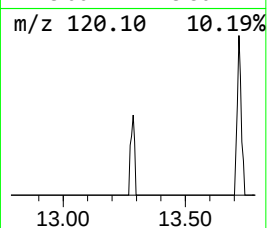
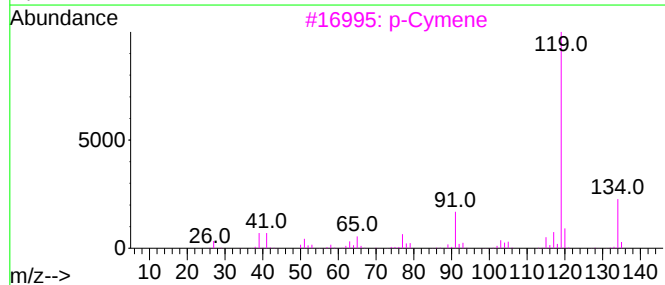
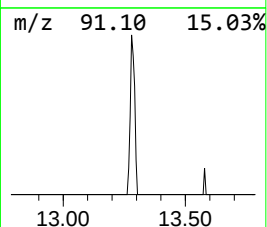
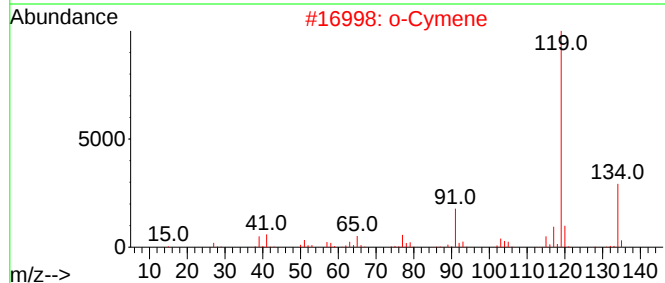
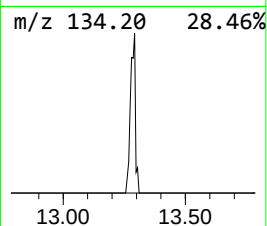
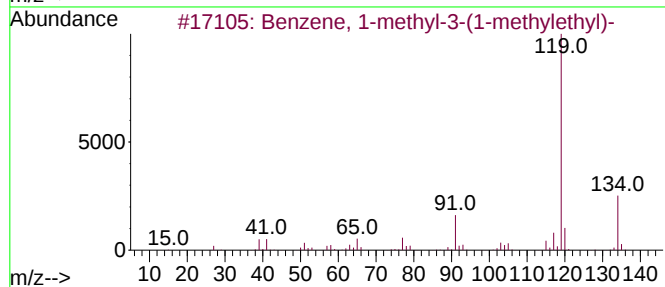
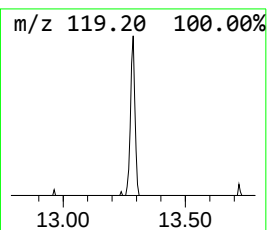
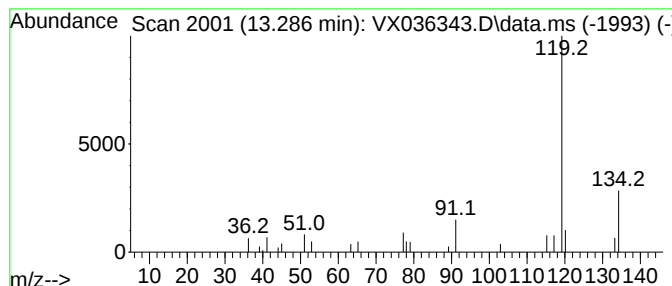
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-methyl-3-(1-meth... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.286	20.12 ug/l	7557	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	91
2			o-Cymene	134	C10H14	000527-84-4	87
3			p-Cymene	134	C10H14	000099-87-6	87
4			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	86
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062723\
Data File : VX036343.D
Acq On : 27 Jun 2023 11:59
Operator : JC/MD
Sample : VX0627MBL01
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VX0627MBL01

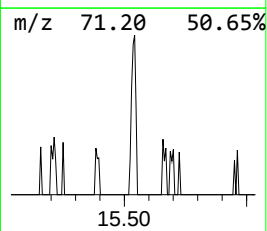
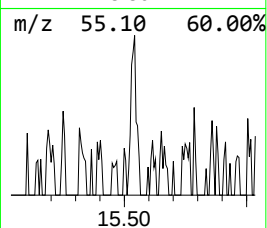
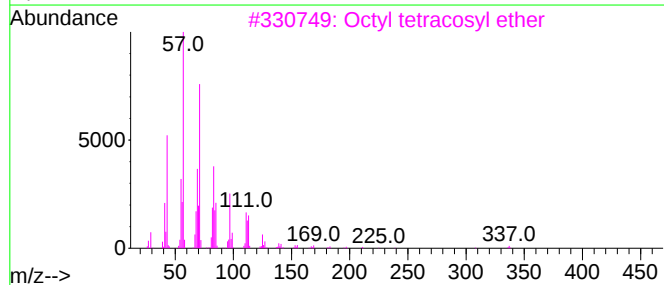
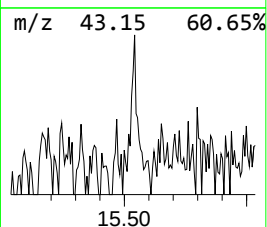
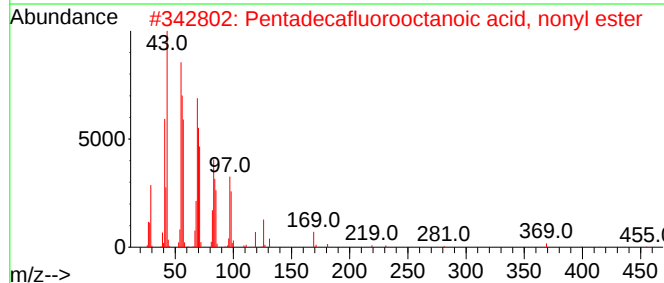
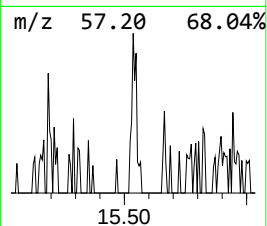
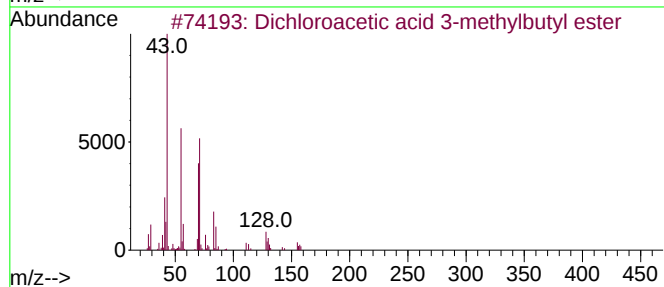
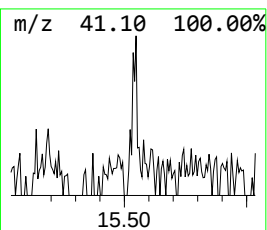
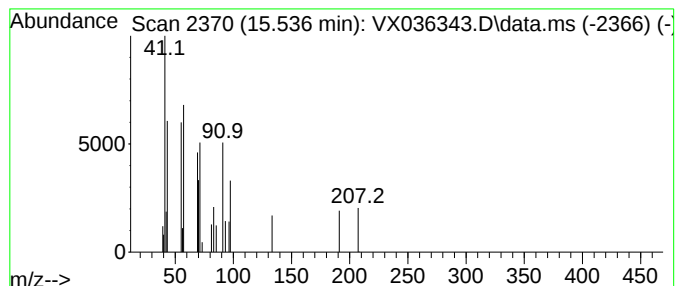
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

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

Peak Number 9 unknown15.536 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.536	14.51 ug/l	5450	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid 3-methylbuty...	198	C7H12Cl2O2	037587-83-0	38
2			Pentadecafluorooctanoic acid, no...	540	C17H19F15O2	1000406-03-9	35
3			Octyl tetracosyl ether	467	C32H66O	1000406-39-0	32
4			Docosyl octyl ether	438	C30H62O	1000406-38-9	32
5			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062723\
Data File : VX036343.D
Acq On : 27 Jun 2023 11:59
Operator : JC/MD
Sample : VX0627MBL01
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VX0627MBL01

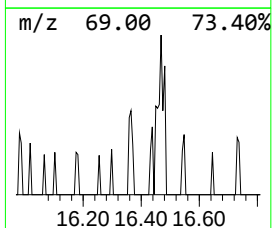
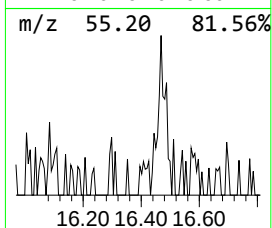
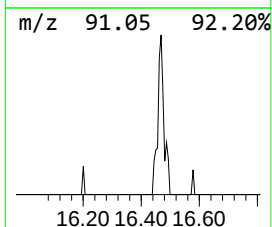
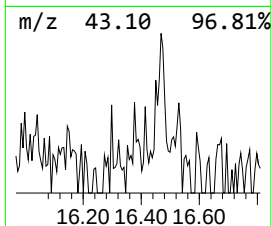
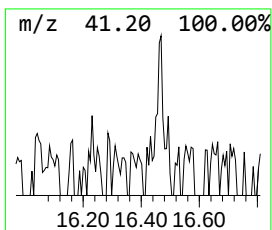
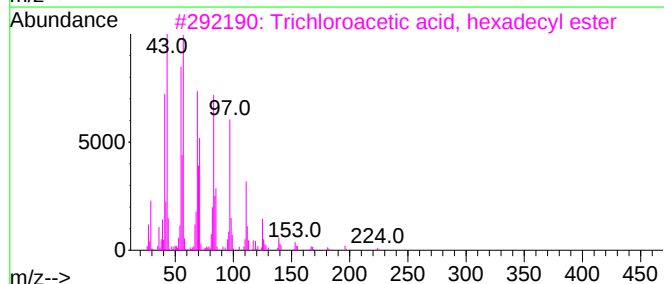
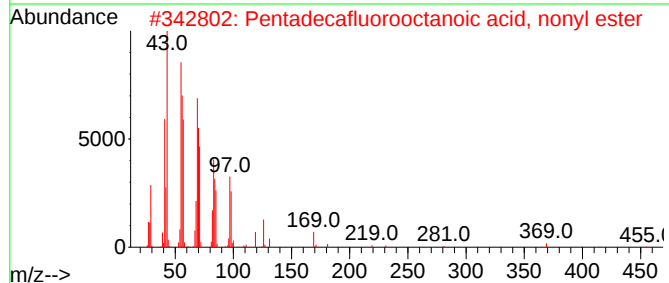
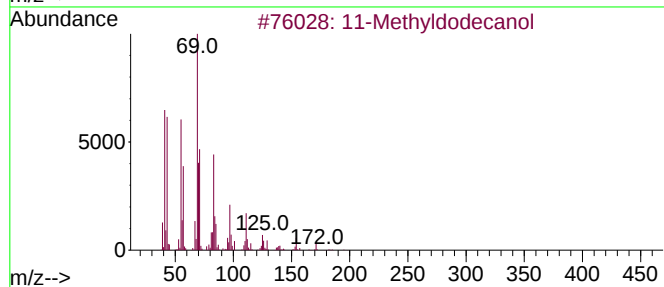
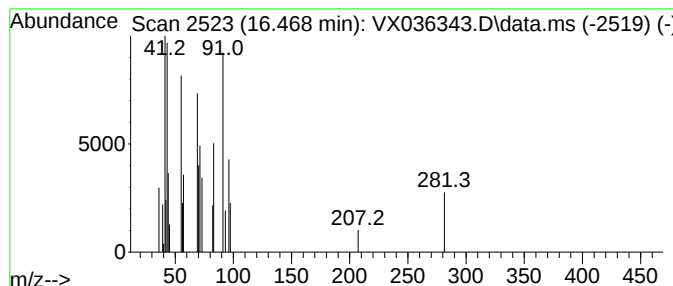
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

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

Peak Number 10 11-Methyldodecanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.468	13.04 ug/l	4895	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11-Methyldodecanol	200	C13H28O	085763-57-1	50
2			Pentadecafluorooctanoic acid, no...	540	C17H19F15O2	1000406-03-9	47
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	47
4			Cyclododecane	168	C12H24	000294-62-2	43
5			3-Heptafluorobutyroxytridecane	396	C17H27F7O2	1000245-49-5	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062723\
Data File : VX036343.D
Acq On : 27 Jun 2023 11:59
Operator : JC/MD
Sample : VX0627MBL01
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VX0627MBL01

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propene	1.142	13.6	ug/l	5209	1	5.544	19186	50.0
unknown3.087	3.087	16.7	ug/l	6398	1	5.544	19186	50.0
Formamide, N-me...	4.580	46.0	ug/l	17669	1	5.544	19186	50.0
Benzene, 1-meth...	13.286	20.1	ug/l	7557	4	12.024	18776	50.0
unknown15.536	15.536	14.5	ug/l	5450	4	12.024	18776	50.0
11-Methyldodecanol	16.468	13.0	ug/l	4895	4	12.024	18776	50.0