

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081523\
 Data File : VX037000.D
 Acq On : 15 Aug 2023 20:08
 Operator : JC/MD
 Sample : 03983-04
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 713-E

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\82X072123W.M
 Title : SW846 8260

Signal : TIC: VX037000.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	6	9	19	rBV	15925	18590	2.43%	0.235%
2	1.453	56	60	72	rBV	102238	122303	15.97%	1.549%
3	2.294	193	198	205	rVB	5458	8795	1.15%	0.111%
4	2.380	205	212	227	rBV	464406	765653	100.00%	9.698%
5	2.538	231	238	244	rBV	21446	39111	5.11%	0.495%
6	2.959	299	307	322	rBV	117010	251783	32.88%	3.189%
7	4.013	468	480	492	rBV2	19923	50891	6.65%	0.645%
8	4.233	504	516	531	rBV2	28930	82476	10.77%	1.045%
9	4.562	560	570	583	rBV	55816	165211	21.58%	2.093%
10	5.001	632	642	660	rBV2	18644	64825	8.47%	0.821%
11	5.391	693	706	720	rBV	84431	248122	32.41%	3.143%
12	5.556	721	733	749	rVB	134448	386385	50.46%	4.894%
13	5.958	788	799	806	rBV	90776	238583	31.16%	3.022%
14	6.037	806	812	822	rVB2	44027	117231	15.31%	1.485%
15	6.330	853	860	877	rVB6	3104	11413	1.49%	0.145%
16	6.641	901	911	920	rBV	6722	17791	2.32%	0.225%
17	6.763	920	931	950	rVB	226532	536819	70.11%	6.800%
18	7.464	1040	1046	1053	rBV2	10680	24332	3.18%	0.308%
19	7.909	1112	1119	1133	rVB3	6251	15011	1.96%	0.190%
20	8.220	1163	1170	1176	rBV	4966	8318	1.09%	0.105%
21	8.433	1195	1205	1209	rBV5	3211	7933	1.04%	0.100%
22	8.574	1222	1228	1234	rBV	39333	67174	8.77%	0.851%
23	8.647	1234	1240	1247	rVV	463528	739251	96.55%	9.364%
24	8.720	1247	1252	1258	rVV	41624	69939	9.13%	0.886%
25	8.805	1262	1266	1271	rVV	7409	13314	1.74%	0.169%
26	8.970	1287	1293	1297	rBV4	5552	10281	1.34%	0.130%
27	9.031	1297	1303	1312	rVB	10213	17801	2.32%	0.225%
28	9.238	1332	1337	1343	rBV	5982	10078	1.32%	0.128%
29	9.445	1365	1371	1375	rBV2	13459	28378	3.71%	0.359%
30	9.488	1375	1378	1381	rVV	14488	21308	2.78%	0.270%
31	9.531	1381	1385	1394	rVV	75666	112348	14.67%	1.423%
32	9.616	1394	1399	1404	rVB2	13066	19461	2.54%	0.247%
33	10.055	1460	1471	1485	rBV	506362	737939	96.38%	9.347%
34	10.195	1488	1494	1500	rBV	28059	42550	5.56%	0.539%
35	10.268	1500	1506	1508	rVV2	22444	31473	4.11%	0.399%
36	10.299	1508	1511	1518	rVB	85104	116591	15.23%	1.477%

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Integrator: RTE

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

Peak separation: 5

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37	10.409	1522	1529	1533	rBV2	13189	24985	3.26%	0.316%
38	10.506	1540	1545	1549	rBV	26338	33945	4.43%	0.430%
39	10.646	1563	1568	1571	rBV2	52562	91041	11.89%	1.153%
40	10.683	1571	1574	1581	rVB	82006	102452	13.38%	1.298%
41	10.756	1581	1586	1587	rBV2	8071	11448	1.50%	0.145%
42	10.854	1599	1602	1606	rVV4	6270	9506	1.24%	0.120%
43	10.896	1606	1609	1614	rVB3	7983	11333	1.48%	0.144%
44	11.079	1634	1639	1645	rBV	422469	537138	70.15%	6.804%
45	11.128	1645	1647	1656	rVV4	11325	24956	3.26%	0.316%
46	11.378	1681	1688	1691	rBV5	6288	11489	1.50%	0.146%
47	11.427	1693	1696	1702	rVV4	6909	12592	1.64%	0.159%
48	11.616	1722	1727	1734	rVB7	7864	18643	2.43%	0.236%
49	11.750	1745	1749	1754	rVB2	16176	21537	2.81%	0.273%
50	11.811	1754	1759	1761	rBV	6232	9370	1.22%	0.119%
51	11.866	1766	1768	1776	rVB5	4697	8522	1.11%	0.108%
52	12.018	1788	1793	1801	rBV	498835	651329	85.07%	8.250%
53	12.085	1801	1804	1809	rVV	9407	13198	1.72%	0.167%
54	12.134	1809	1812	1820	rVB7	5030	8367	1.09%	0.106%
55	12.219	1820	1826	1838	rBV	346686	509607	66.56%	6.455%
56	12.311	1839	1841	1852	rVV8	9676	24168	3.16%	0.306%
57	12.414	1853	1858	1863	rVV	58952	78379	10.24%	0.993%
58	12.488	1866	1870	1874	rVB	10312	13321	1.74%	0.169%
59	12.805	1913	1922	1927	rBV2	28648	57986	7.57%	0.734%
60	13.426	2020	2024	2029	rVB3	9147	13359	1.74%	0.169%
61	13.579	2046	2049	2057	rBV6	4745	10644	1.39%	0.135%
62	13.713	2067	2071	2075	rVV2	5837	8695	1.14%	0.110%
63	13.774	2075	2081	2087	rVB	137987	175944	22.98%	2.229%
64	13.865	2093	2096	2101	rVB	7679	11423	1.49%	0.145%
65	14.225	2146	2155	2161	rBV6	5328	11641	1.52%	0.147%
66	14.481	2192	2197	2201	rBV2	6887	9952	1.30%	0.126%
67	14.633	2215	2222	2227	rBV	28411	42612	5.57%	0.540%
68	14.780	2240	2246	2250	rBV	15422	21207	2.77%	0.269%
69	15.207	2313	2316	2320	rVB2	6191	7705	1.01%	0.098%
70	15.371	2338	2343	2349	rBV	7417	10972	1.43%	0.139%
71	15.475	2353	2360	2364	rBV3	8410	14511	1.90%	0.184%
72	15.615	2378	2383	2386	rBV3	8861	14070	1.84%	0.178%
73	15.835	2411	2419	2429	rBV7	3250	9219	1.20%	0.117%
74	15.975	2437	2442	2449	rBV7	3490	8662	1.13%	0.110%
75	16.328	2493	2500	2509	rBV3	8117	19509	2.55%	0.247%

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Instrument :
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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\82X072123W.M
Title : SW846 8260

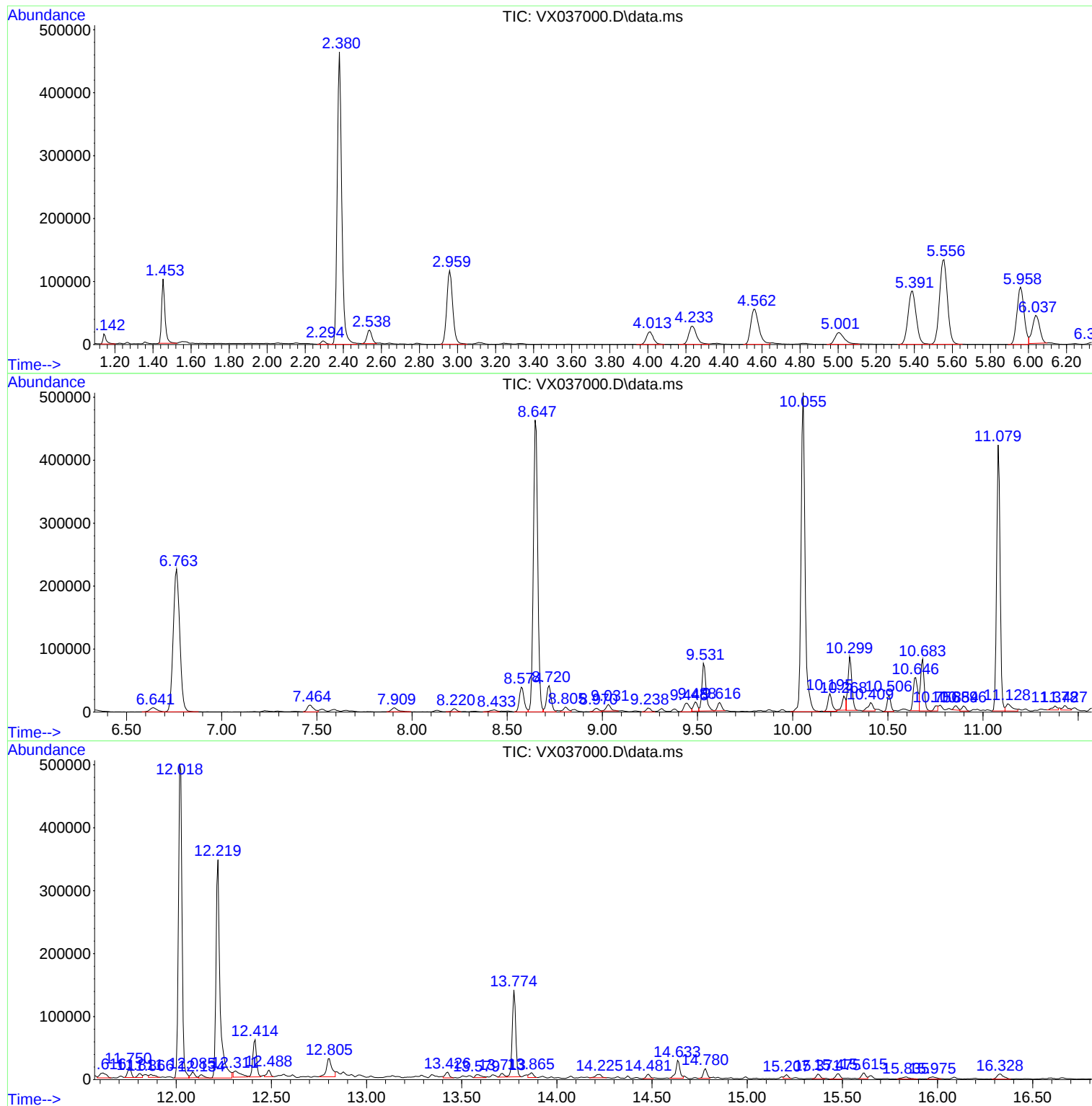
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Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081523\
Data File : VX037000.D
Acq On : 15 Aug 2023 20:08
Operator : JC/MD
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Instrument :
MSVOA_X
ClientSampleId :
713-E

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081523\
Data File : VX037000.D
Acq On : 15 Aug 2023 20:08
Operator : JC/MD
Sample : 03983-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
713-E

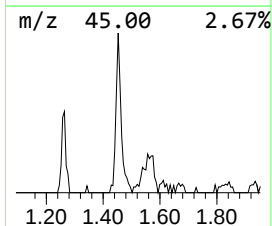
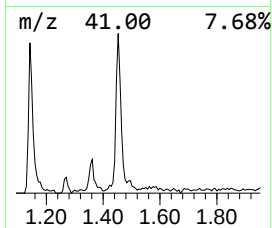
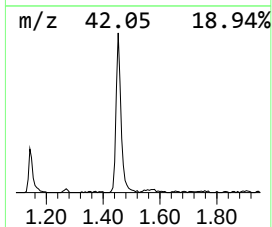
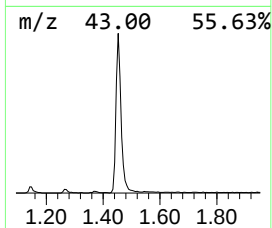
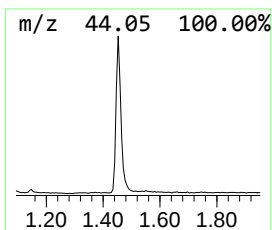
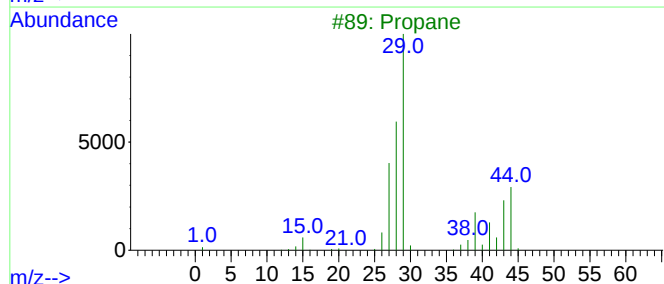
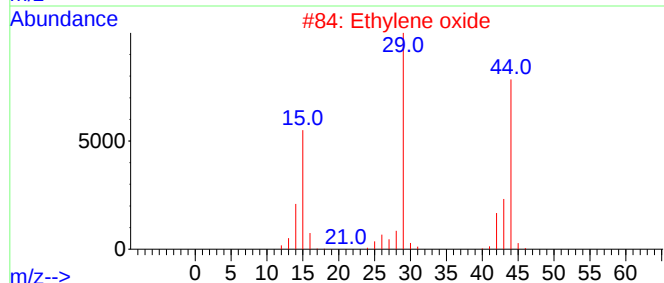
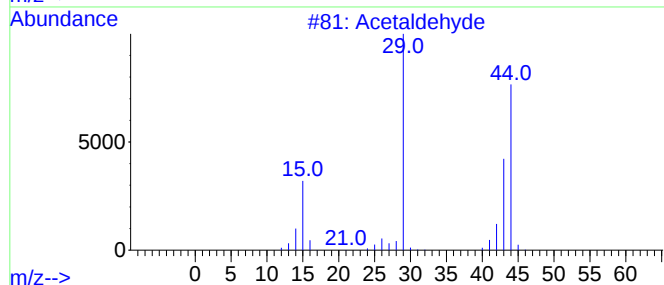
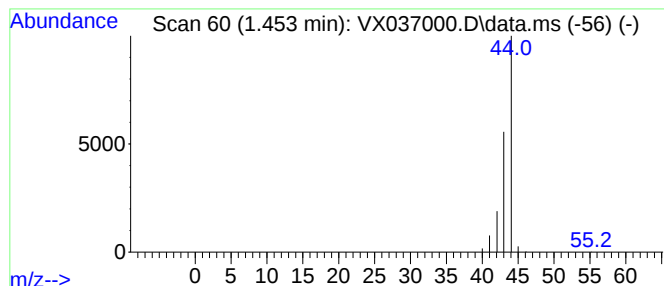
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.453	15.83 ug/l	122303	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
2			Ethylene oxide	44	C2H4O	000075-21-8	5
3			Propane	44	C3H8	000074-98-6	4
4			Alanine	89	C3H7NO2	000056-41-7	4
5			Hydrogen isocyanate	43	CHNO	000075-13-8	3



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Instrument :
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ClientSampleId :
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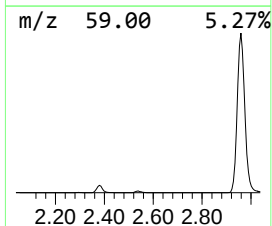
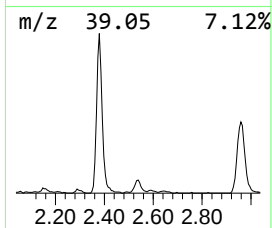
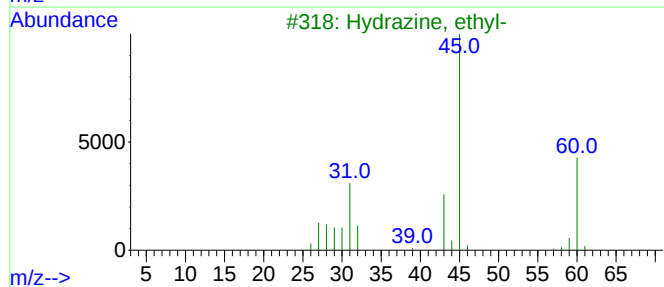
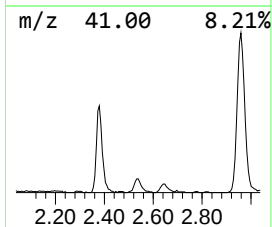
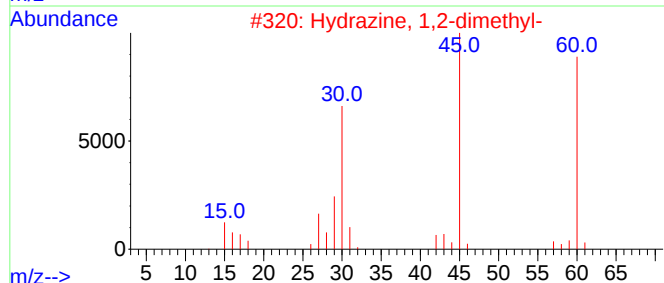
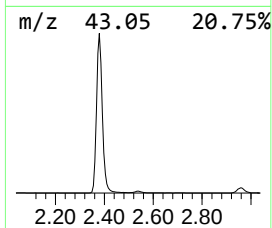
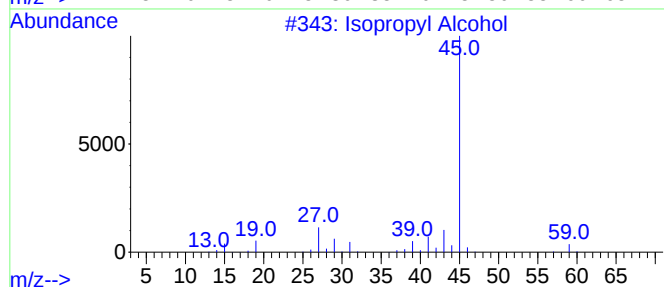
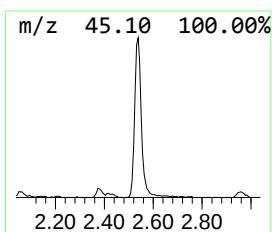
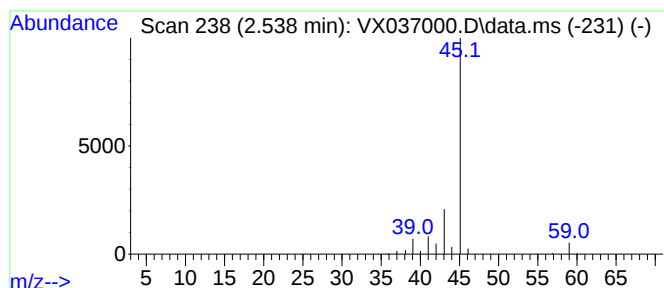
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.538	5.06 ug/l	39111	Pentafluorobenzene	5.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2		Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
3		Hydrazine, ethyl-	60	C2H8N2	000624-80-6	9
4		Formamide	45	CH3NO	000075-12-7	5
5		Ethylamine	45	C2H7N	000075-04-7	4



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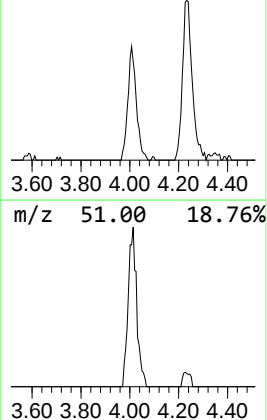
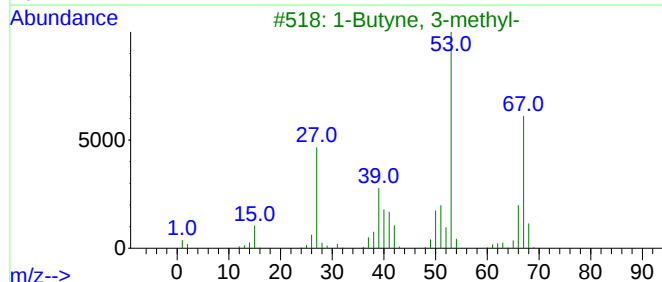
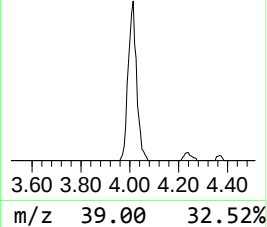
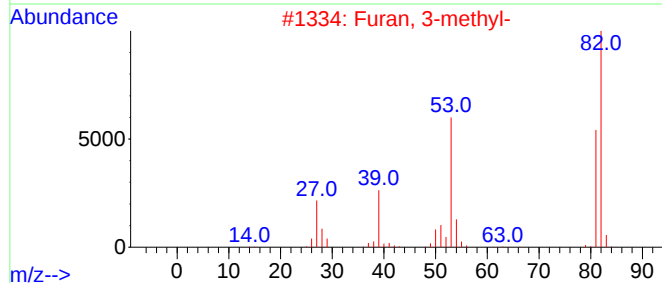
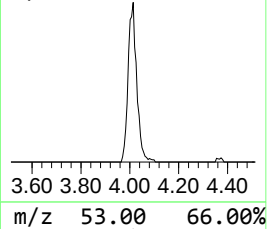
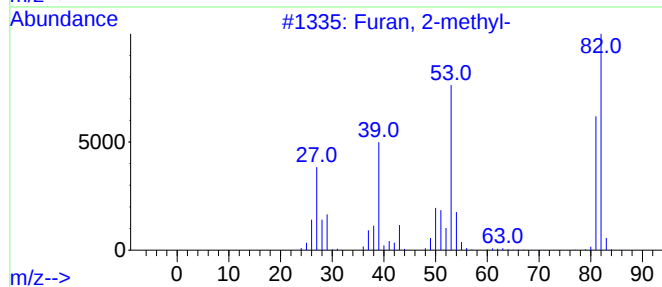
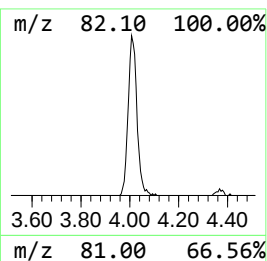
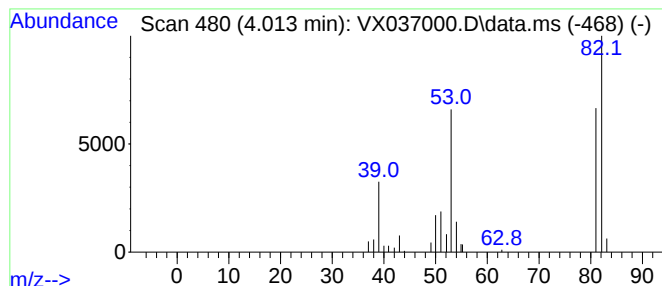
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 3 Furan, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.013	6.59 ug/l	50891	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, 2-methyl-	82	C5H6O	000534-22-5	91
2			Furan, 3-methyl-	82	C5H6O	000930-27-8	90
3			1-Butyne, 3-methyl-	68	C5H8	000598-23-2	50
4			1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	35
5			1H-Pyrazole, 1-methyl-	82	C4H6N2	000930-36-9	22



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Instrument :
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ClientSampleId :
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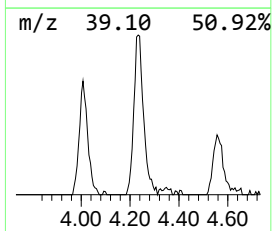
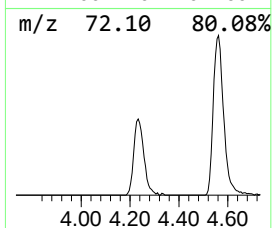
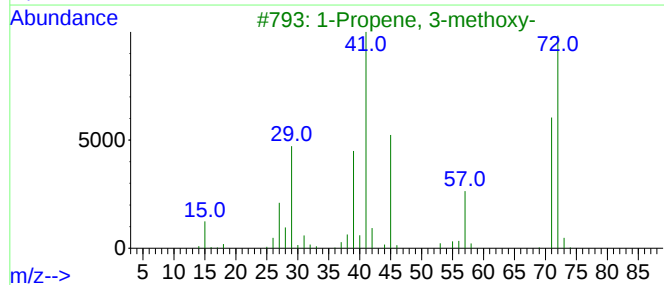
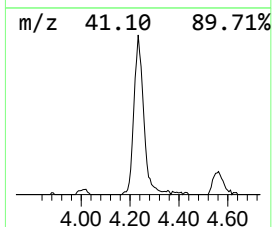
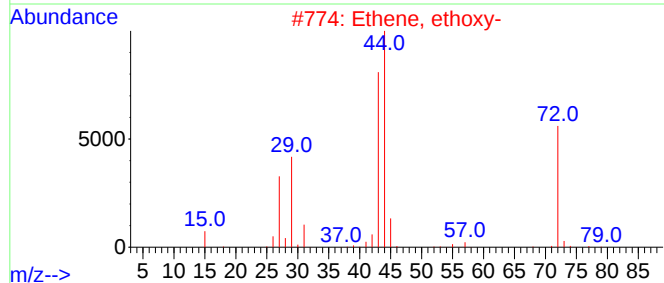
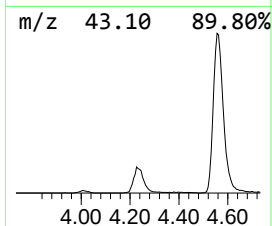
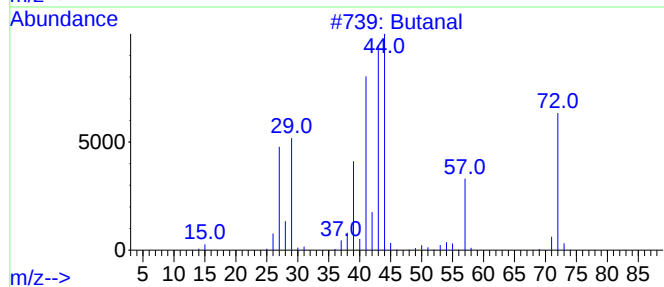
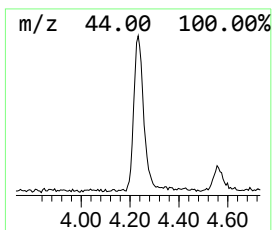
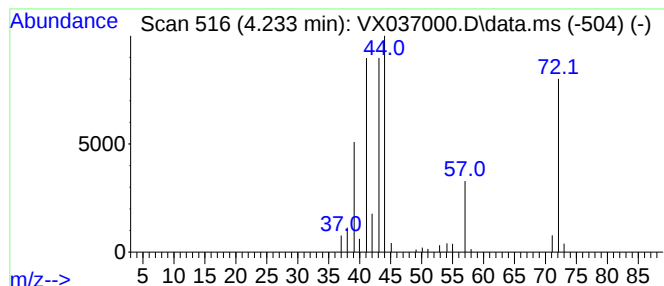
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 4 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.233	10.67 ug/l	82476	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	94
2			Ethene, ethoxy-	72	C4H8O	000109-92-2	53
3			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	47
4			Propane	44	C3H8	000074-98-6	47
5			Propanal, 2-methyl-	72	C4H8O	000078-84-2	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081523\
Data File : VX037000.D
Acq On : 15 Aug 2023 20:08
Operator : JC/MD
Sample : 03983-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
713-E

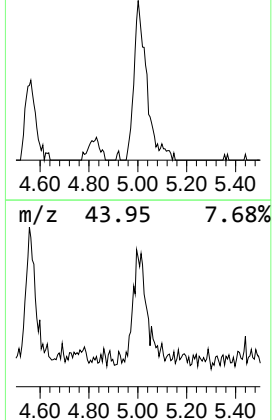
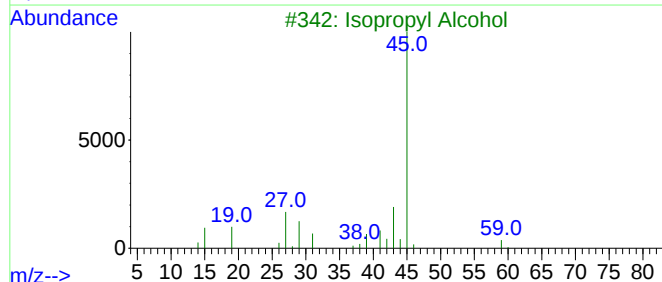
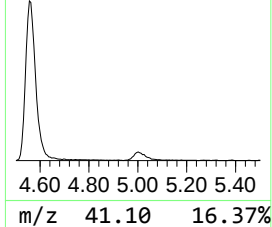
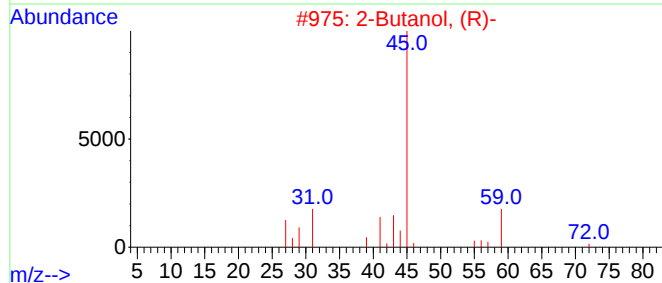
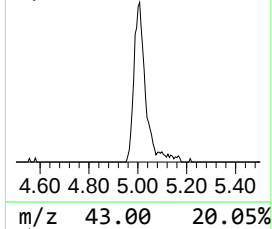
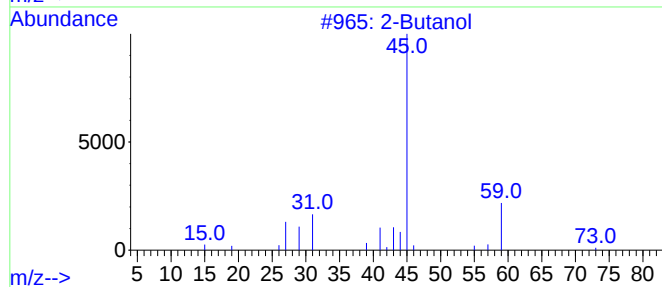
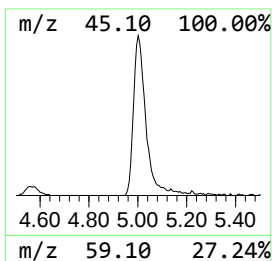
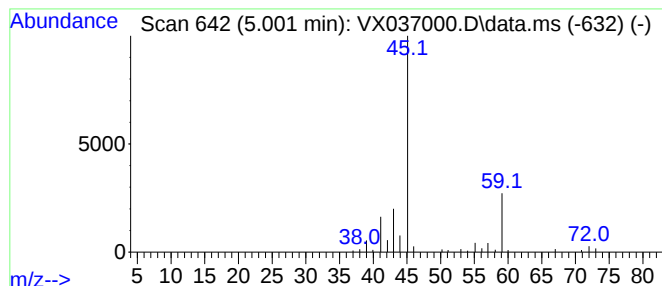
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Quant Title : SW846 8260

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

Peak Number 5 2-Butanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.001	8.39 ug/l	64825	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butanol	74	C4H10O	000078-92-2	83
2			2-Butanol, (R)-	74	C4H10O	014898-79-4	83
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	59
4			2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	45
5			2-Hexanol, (R)-	102	C6H14O	026549-24-6	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081523\
Data File : VX037000.D
Acq On : 15 Aug 2023 20:08
Operator : JC/MD
Sample : 03983-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
713-E

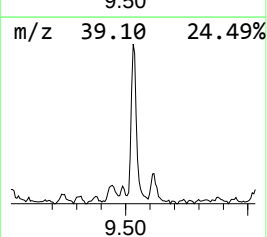
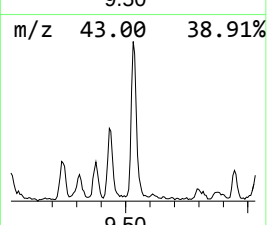
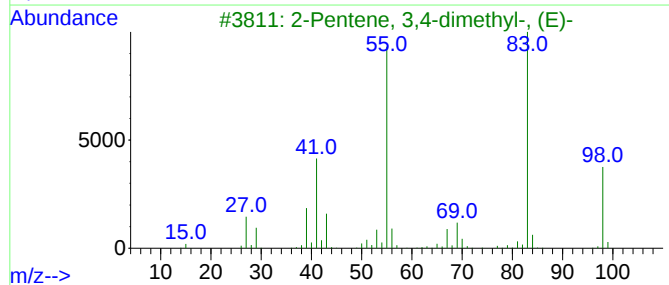
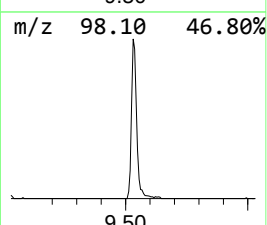
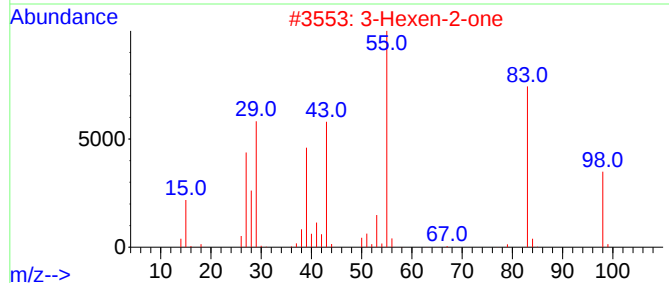
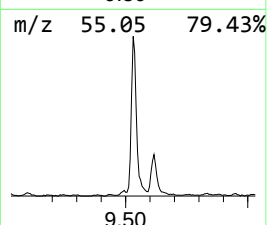
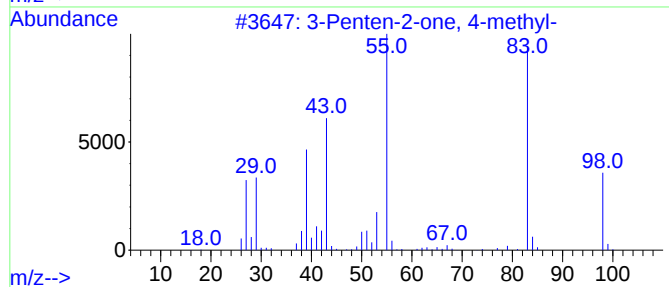
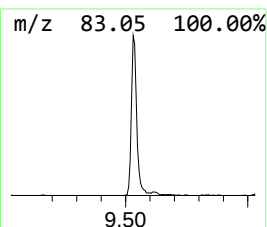
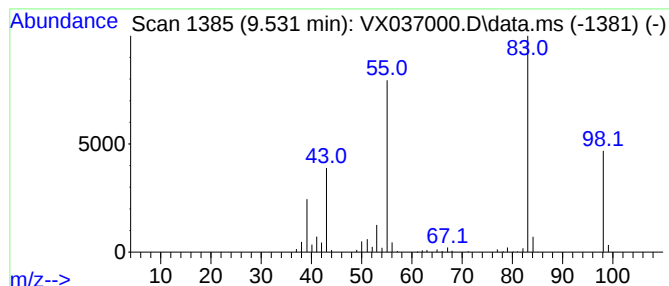
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Quant Title : SW846 8260

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

Peak Number 6 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.531	7.61 ug/l	112348	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4			Cyclohexane, methyl-	98	C7H14	000108-87-2	80
5			Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081523\
Data File : VX037000.D
Acq On : 15 Aug 2023 20:08
Operator : JC/MD
Sample : 03983-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
713-E

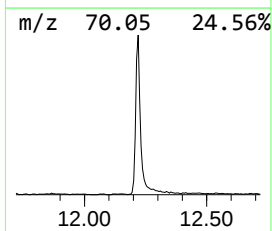
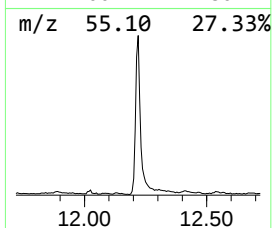
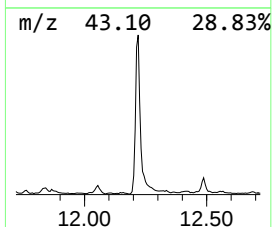
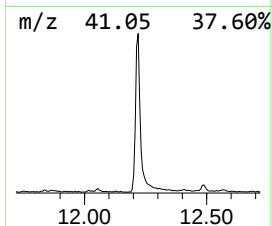
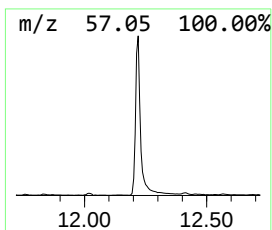
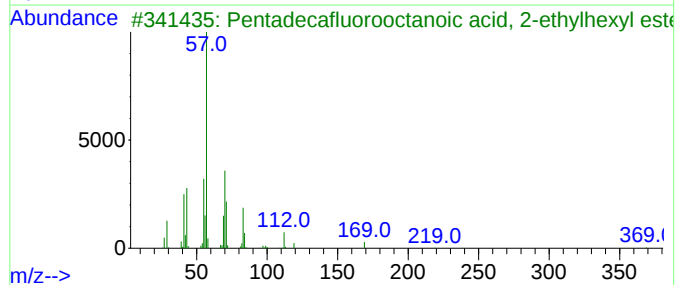
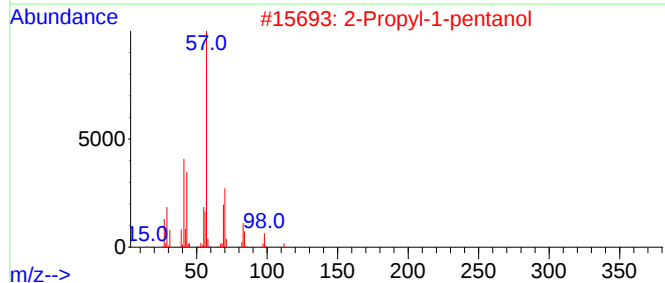
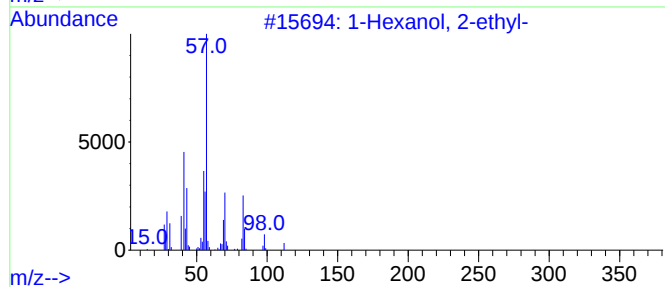
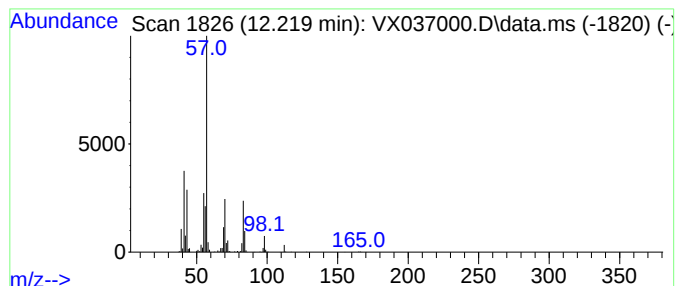
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Quant Title : SW846 8260

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

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	39.12 ug/l	509607	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	53
4			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5			2-Ethyl-1-hexanol, pentafluoropr...	276	C11H17F5O2	959012-82-9	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081523\
Data File : VX037000.D
Acq On : 15 Aug 2023 20:08
Operator : JC/MD
Sample : 03983-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
713-E

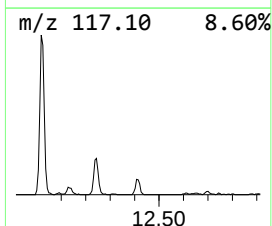
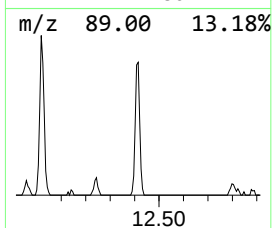
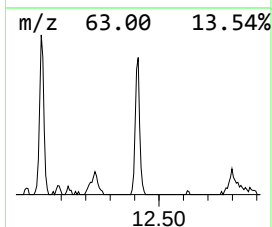
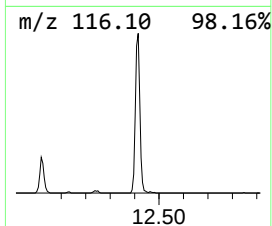
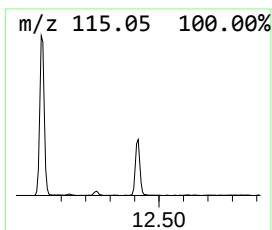
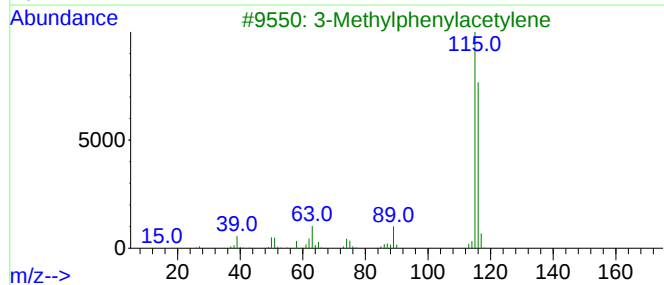
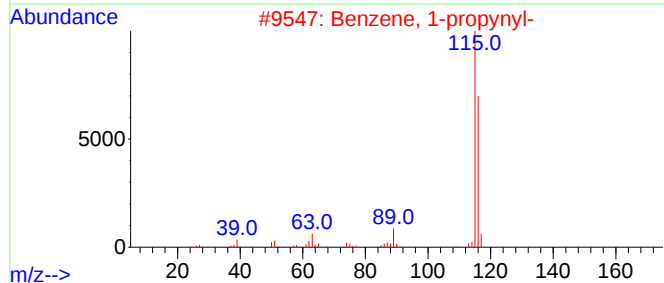
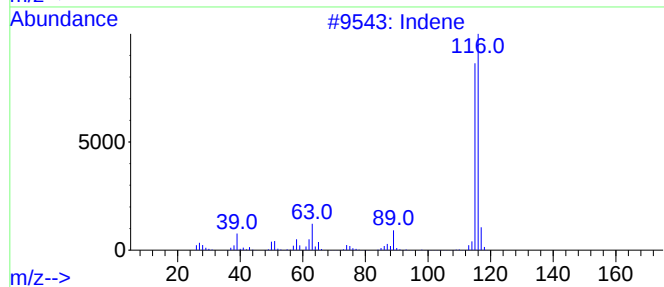
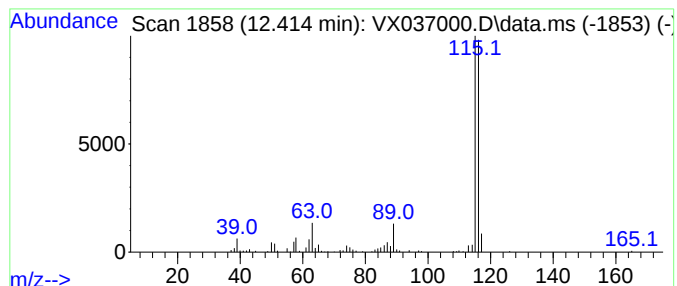
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 8 Indene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.414	6.02 ug/l	78379	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	96
2			Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
3			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	90
5			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081523\
Data File : VX037000.D
Acq On : 15 Aug 2023 20:08
Operator : JC/MD
Sample : 03983-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
713-E

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	1.453	15.8	ug/l	122303	1	5.556	386385	50.0
Isopropyl Alcohol	2.538	5.1	ug/l	39111	1	5.556	386385	50.0
Furan, 2-methyl-	4.013	6.6	ug/l	50891	1	5.556	386385	50.0
Butanal	4.233	10.7	ug/l	82476	1	5.556	386385	50.0
2-Butanol	5.001	8.4	ug/l	64825	1	5.556	386385	50.0
3-Penten-2-one,...	9.531	7.6	ug/l	112348	3	10.055	737939	50.0
1-Hexanol, 2-et...	12.219	39.1	ug/l	509607	4	12.024	651329	50.0
Indene	12.414	6.0	ug/l	78379	4	12.024	651329	50.0