

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122823\
 Data File : VX039509.D
 Acq On : 28 Dec 2023 12:29
 Operator : JC/MD
 Sample : 06024-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1222

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\82X121323W.M
 Title : SW846 8260

Signal : TIC: VX039509.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	26	29	40	rVB	48000	51616	7.99%	0.750%
2	1.367	41	46	53	rBV	296806	312126	48.31%	4.534%
3	1.428	53	56	59	rVB	16459	15922	2.46%	0.231%
4	1.495	63	67	70	rBV	20638	20813	3.22%	0.302%
5	1.562	71	78	79	rBV5	6130	11388	1.76%	0.165%
6	1.629	88	89	99	rVB3	12376	12390	1.92%	0.180%
7	1.727	100	105	116	rVB	148415	209953	32.49%	3.050%
8	1.898	128	133	136	rBV	7072	9969	1.54%	0.145%
9	1.946	136	141	154	rVV2	56257	99429	15.39%	1.444%
10	2.062	154	160	169	rVV2	36034	79936	12.37%	1.161%
11	2.154	170	175	179	rVV	15353	25391	3.93%	0.369%
12	2.209	179	184	195	rVV	39116	63547	9.83%	0.923%
13	2.337	199	205	208	rVV2	4902	8973	1.39%	0.130%
14	2.385	208	213	221	rVB	7539	13176	2.04%	0.191%
15	2.745	260	272	275	rBV	10288	22832	3.53%	0.332%
16	2.818	280	284	287	rVV	16799	31686	4.90%	0.460%
17	2.861	287	291	301	rVB	18615	39279	6.08%	0.571%
18	3.099	323	330	341	rVB2	11595	27088	4.19%	0.394%
19	3.440	379	386	394	rBV3	6923	16476	2.55%	0.239%
20	4.300	518	527	539	rVB2	16853	46865	7.25%	0.681%
21	5.385	693	705	715	rBV3	69553	208680	32.30%	3.032%
22	5.470	715	719	724	rVV4	11245	30176	4.67%	0.438%
23	5.549	724	732	752	rVB	104283	306489	47.43%	4.452%
24	5.818	769	776	787	rBV6	2648	8812	1.36%	0.128%
25	5.958	787	799	805	rBV	81177	217307	33.63%	3.157%
26	6.037	805	812	825	rVB	110618	295132	45.68%	4.287%
27	6.244	838	846	857	rVB4	6500	20072	3.11%	0.292%
28	6.756	922	930	953	rVB	191894	466287	72.16%	6.774%
29	7.378	1021	1032	1041	rBV3	8980	21928	3.39%	0.319%
30	8.646	1234	1240	1246	rVV	416403	644903	99.81%	9.369%
31	8.720	1246	1252	1265	rVB	401212	646141	100.00%	9.387%
32	10.055	1465	1471	1479	rBV	425700	597642	92.49%	8.682%
33	10.195	1488	1494	1502	rBV	39514	54475	8.43%	0.791%
34	10.299	1504	1511	1521	rBV	136428	186696	28.89%	2.712%
35	10.640	1561	1567	1576	rBV	69167	92473	14.31%	1.343%
36	11.079	1634	1639	1651	rBV	350958	448260	69.37%	6.512%

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37	11.304	1672	1676	1682	rVB	8506	12058	1.87%	0.175%
38	11.378	1682	1688	1696	rBV	32724	60535	9.37%	0.879%
39	11.451	1696	1700	1710	rVB	18553	25235	3.91%	0.367%
40	11.615	1721	1727	1735	rBV	18713	26038	4.03%	0.378%
41	11.749	1744	1749	1757	rVB	49034	64289	9.95%	0.934%
42	12.024	1788	1794	1800	rBV	397005	515846	79.83%	7.494%
43	12.085	1800	1804	1810	rVB	23279	30554	4.73%	0.444%
44	12.243	1822	1830	1838	rBV3	23374	50665	7.84%	0.736%
45	12.316	1838	1842	1851	rVB3	16200	26588	4.11%	0.386%
46	12.463	1863	1866	1871	rVB	6204	7939	1.23%	0.115%
47	12.530	1873	1877	1879	rBV2	6397	8084	1.25%	0.117%
48	12.609	1886	1890	1894	rBV	12124	16200	2.51%	0.235%
49	12.701	1900	1905	1913	rBV3	10635	21842	3.38%	0.317%
50	12.847	1925	1929	1935	rVB3	4506	6636	1.03%	0.096%
51	12.920	1936	1941	1944	rVV2	7494	8952	1.39%	0.130%
52	12.963	1944	1948	1953	rVB	13195	17489	2.71%	0.254%
53	13.048	1954	1962	1964	rBV4	4481	8576	1.33%	0.125%
54	13.170	1978	1982	1986	rVB2	10095	13725	2.12%	0.199%
55	13.292	1992	2002	2007	rBV3	33987	60240	9.32%	0.875%
56	13.420	2019	2023	2032	rVB	26666	38010	5.88%	0.552%
57	13.542	2040	2043	2046	rVV2	7802	9638	1.49%	0.140%
58	13.585	2046	2050	2056	rVV4	11203	23384	3.62%	0.340%
59	13.664	2060	2063	2071	rVB7	8605	14413	2.23%	0.209%
60	13.780	2078	2082	2088	rVB2	5296	10035	1.55%	0.146%
61	13.853	2088	2094	2099	rVB3	11570	20294	3.14%	0.295%
62	13.926	2099	2106	2110	rBV3	13971	20510	3.17%	0.298%
63	14.036	2120	2124	2127	rVB2	10404	10784	1.67%	0.157%
64	14.072	2127	2130	2135	rBV	9452	12206	1.89%	0.177%
65	14.225	2146	2155	2160	rBV2	25261	47061	7.28%	0.684%
66	14.316	2167	2170	2175	rBV5	5478	6924	1.07%	0.101%
67	14.371	2175	2179	2184	rBV2	13018	16168	2.50%	0.235%
68	14.481	2192	2197	2207	rBV4	23583	35923	5.56%	0.522%
69	14.566	2207	2211	2215	rBV5	3788	7625	1.18%	0.111%
70	14.615	2215	2219	2221	rBV2	16404	21340	3.30%	0.310%
71	14.670	2226	2228	2233	rVB2	8712	11192	1.73%	0.163%
72	14.755	2239	2242	2244	rBV	18241	17163	2.66%	0.249%
73	14.779	2244	2246	2250	rVB2	5243	6688	1.04%	0.097%
74	14.901	2263	2266	2273	rVB6	4974	9770	1.51%	0.142%
75	15.103	2295	2299	2302	rBV5	4852	7123	1.10%	0.103%
76	15.182	2308	2312	2314	rBV2	13514	19460	3.01%	0.283%

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Title : SW846 8260

77	15.212	2314	2317	2321	rVV2	18407	24029	3.72%	0.349%
78	15.371	2339	2343	2348	rBV8	6293	10487	1.62%	0.152%
79	15.487	2356	2362	2368	rBV2	30988	51928	8.04%	0.754%
80	15.615	2379	2383	2386	rBV5	8823	14494	2.24%	0.211%
81	15.645	2386	2388	2396	rVB6	8894	15897	2.46%	0.231%
82	16.029	2449	2451	2456	rVB7	5304	7039	1.09%	0.102%
83	16.090	2456	2461	2466	rBV6	9511	20007	3.10%	0.291%
84	16.377	2502	2508	2513	rVB4	14262	28208	4.37%	0.410%

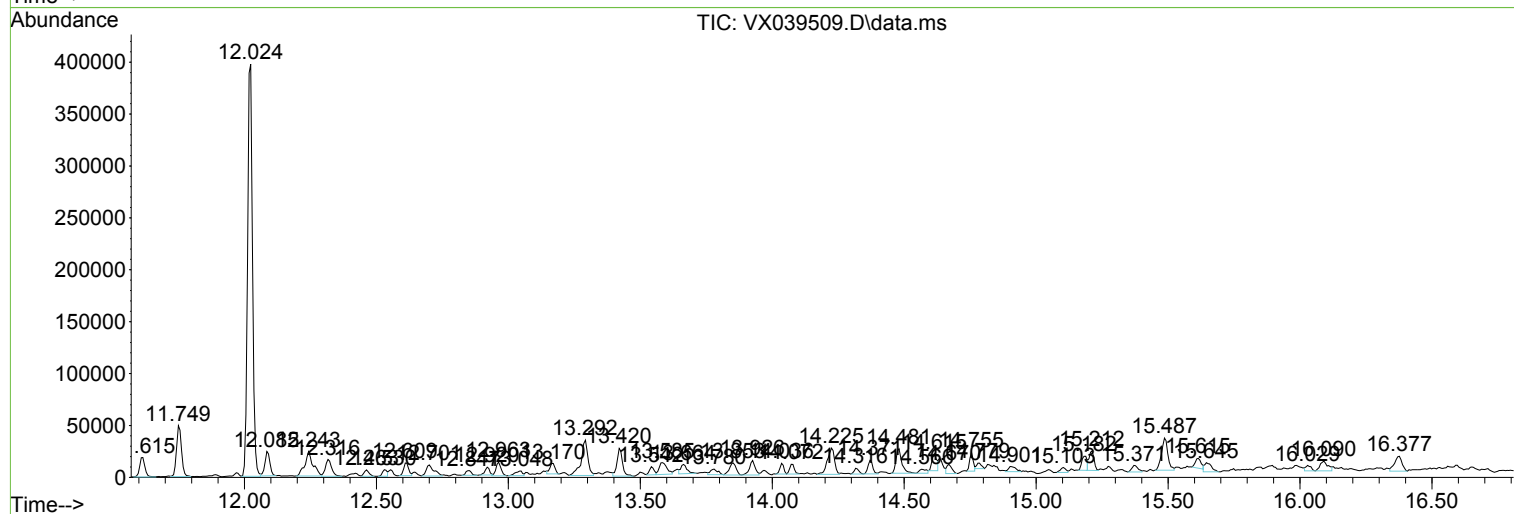
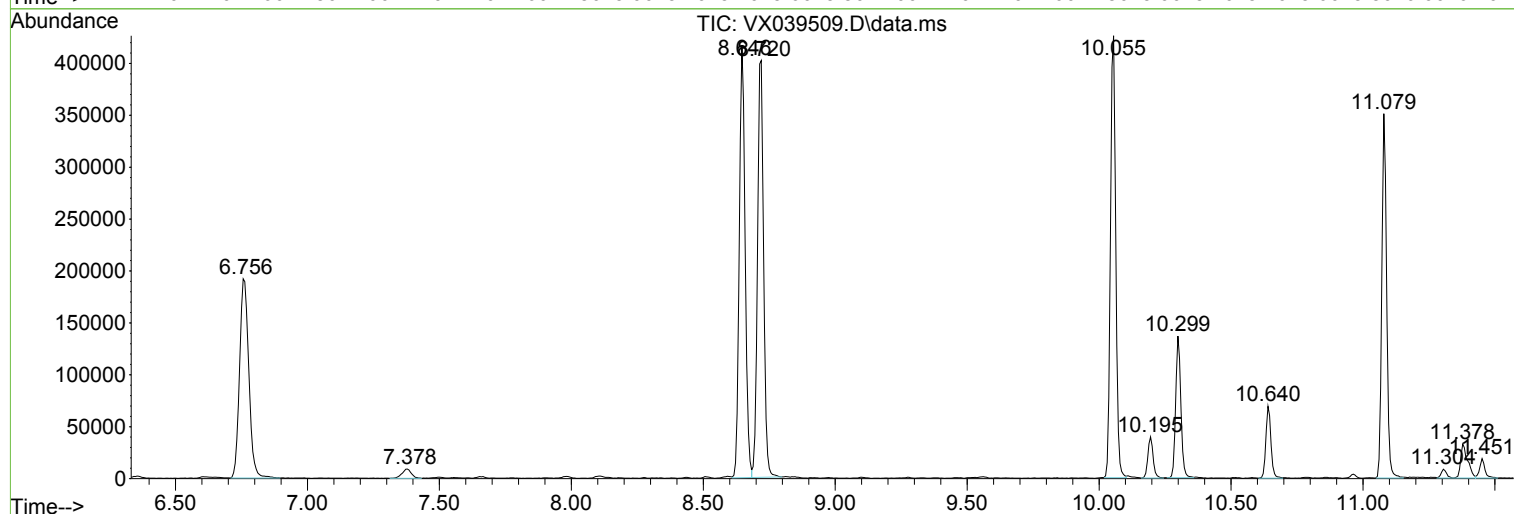
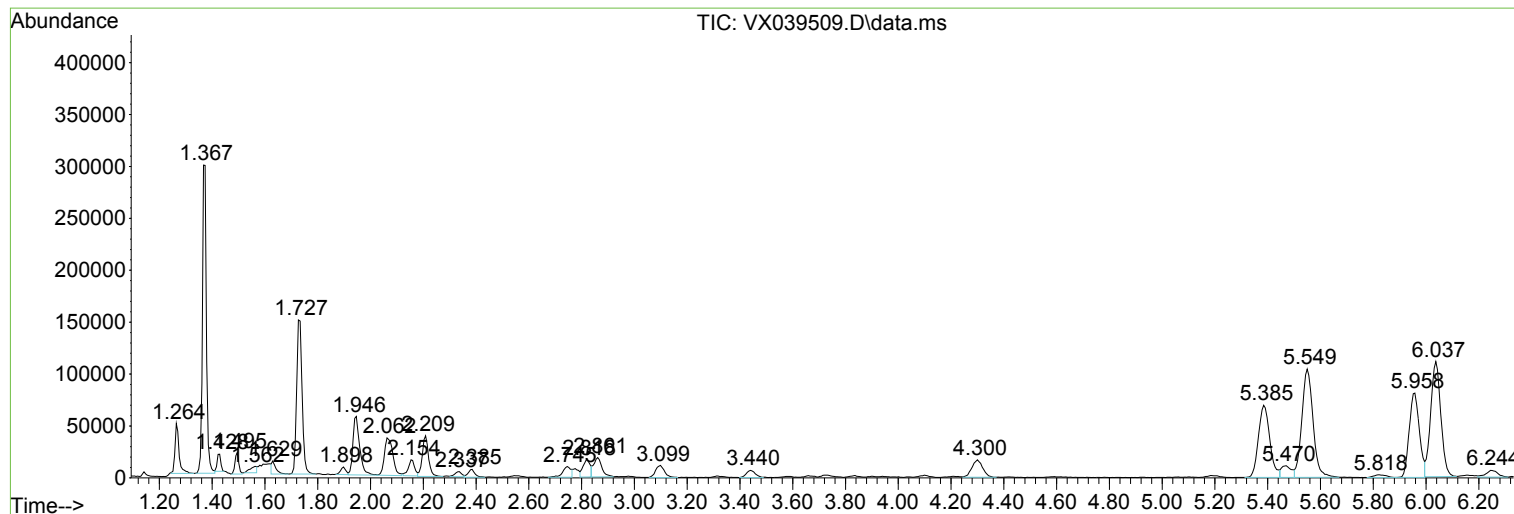
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122823\
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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
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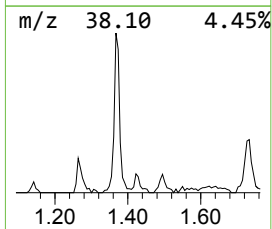
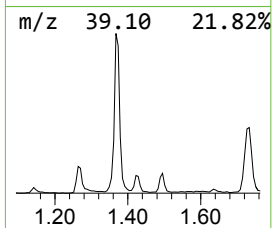
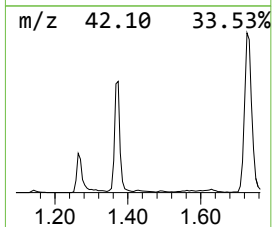
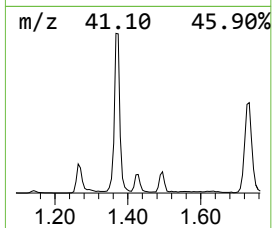
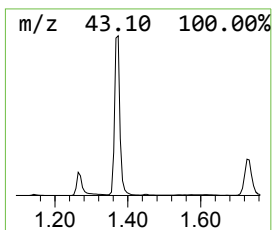
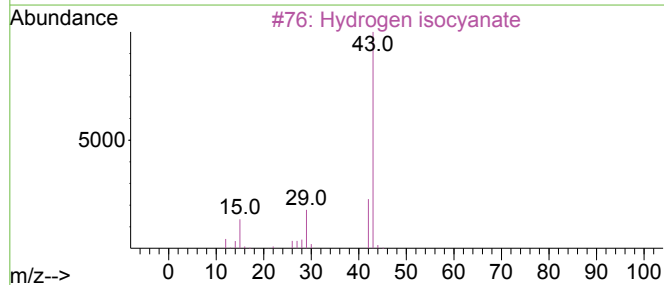
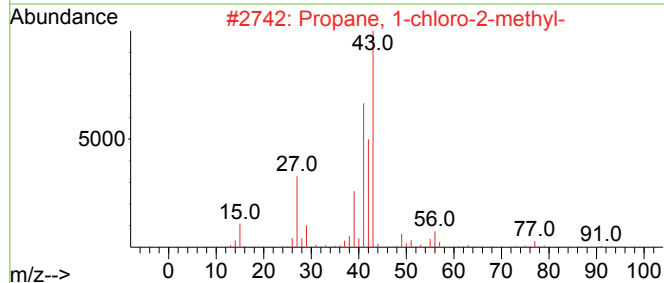
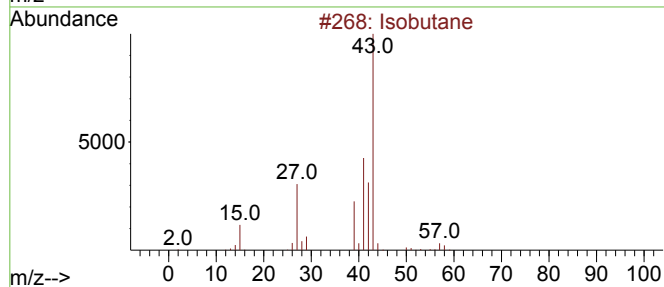
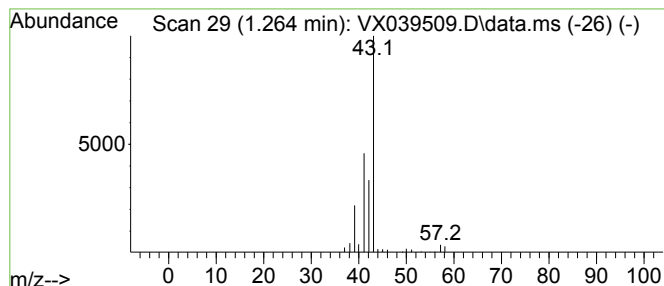
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 1 Isobutane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	8.42 ug/l	51616	Pentafluorobenzene	5.549

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutane	58	C4H10	000075-28-5	64
2			Propane, 1-chloro-2-methyl-	92	C4H9Cl	000513-36-0	9
3			Hydrogen isocyanate	43	CHNO	000075-13-8	4
4			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	4
5			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	2



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Instrument :
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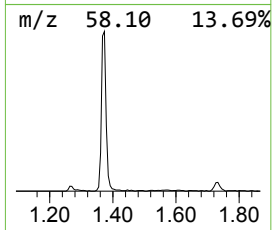
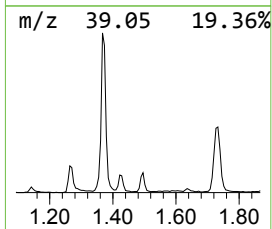
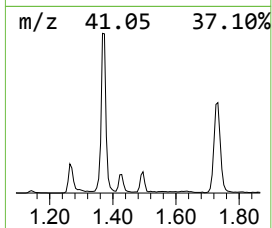
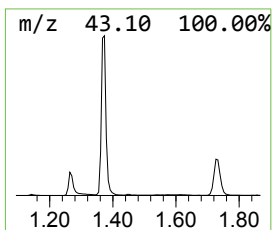
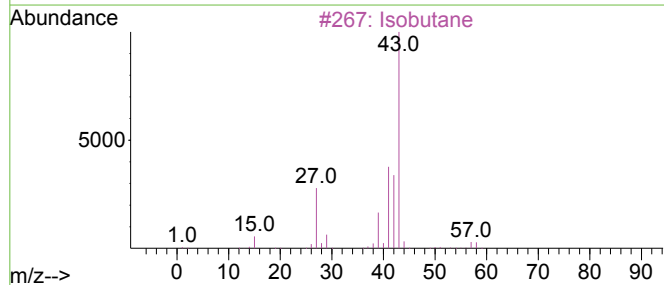
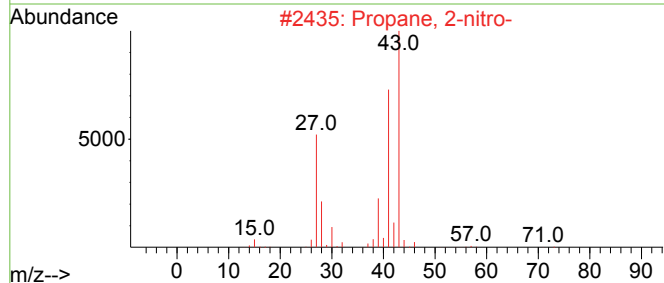
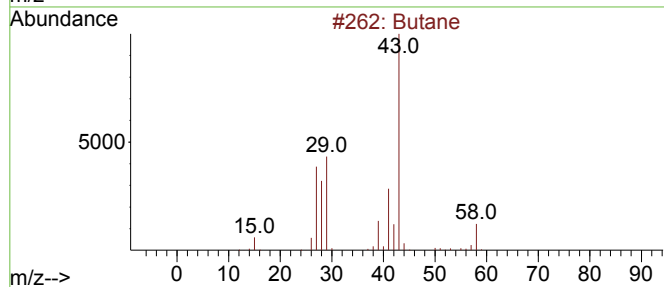
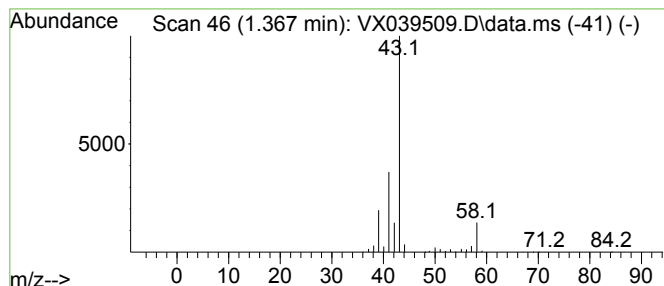
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.367	50.92 ug/l	312126	Pentafluorobenzene	5.549

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	80
2			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	9
3			Isobutane	58	C4H10	000075-28-5	9
4			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9



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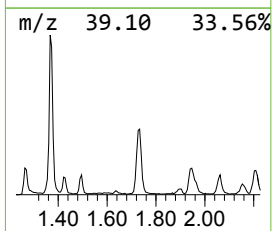
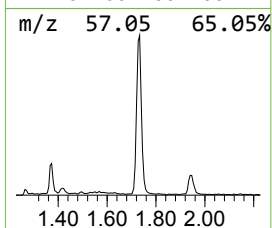
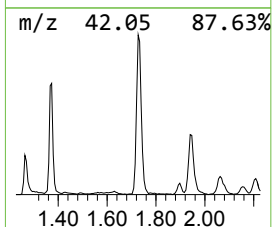
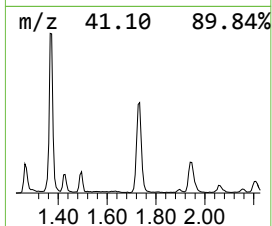
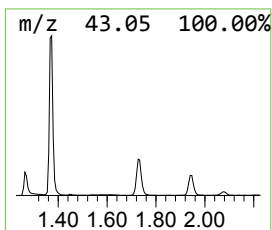
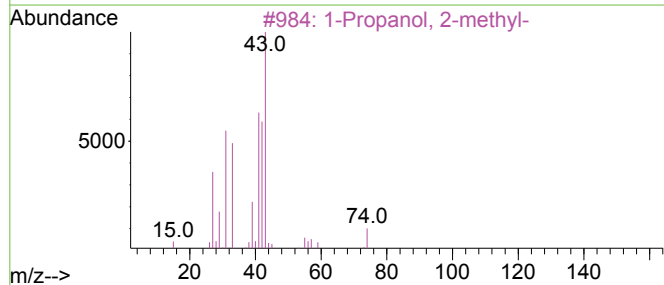
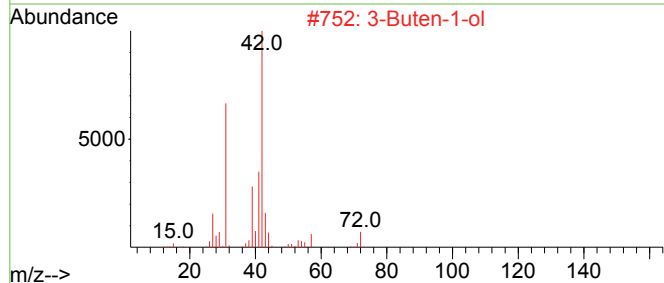
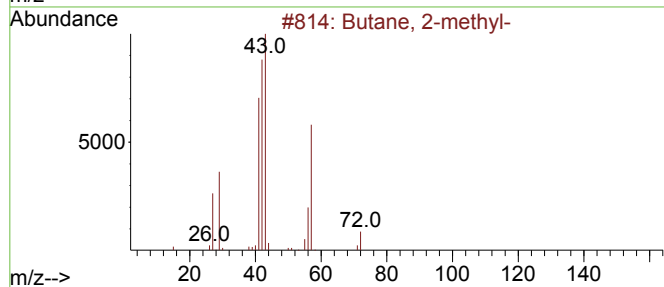
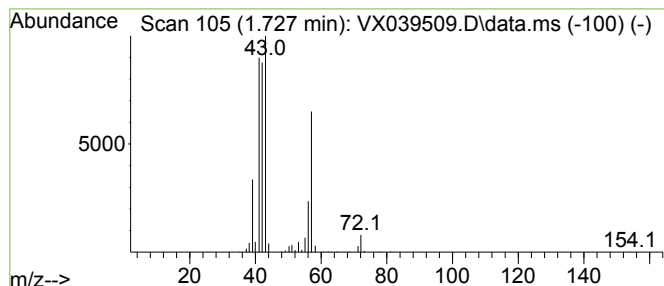
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 3 Butane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.727	34.25 ug/l	209953	Pentafluorobenzene	5.549

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	90
2			3-Buten-1-ol	72	C4H8O	000627-27-0	47
3			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	38
4			Pentane	72	C5H12	000109-66-0	36
5			2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	33



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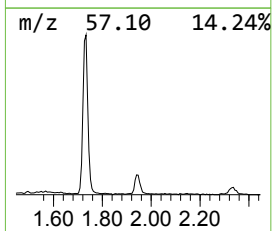
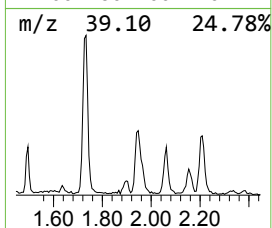
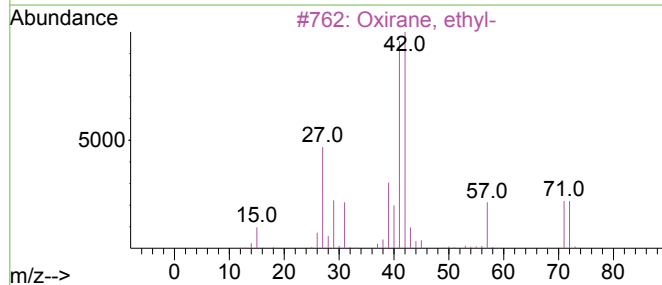
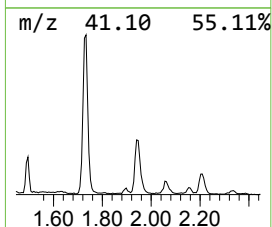
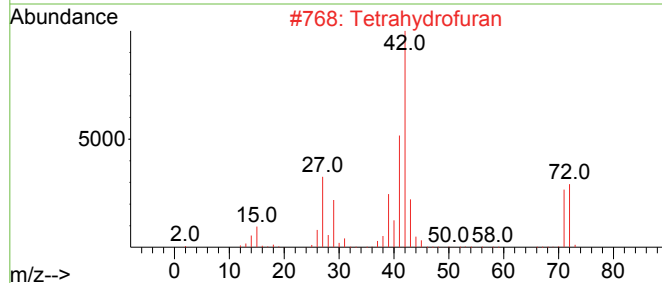
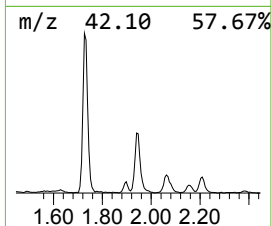
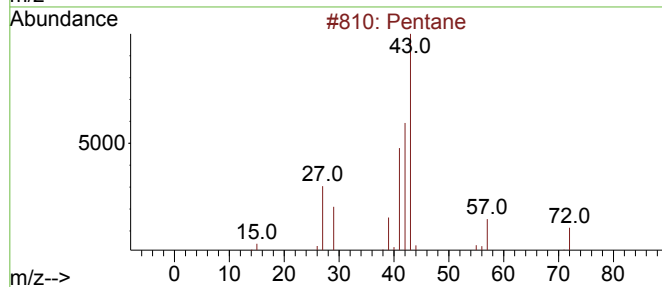
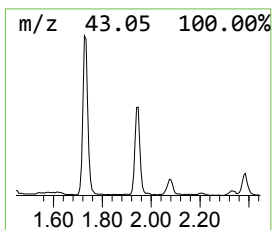
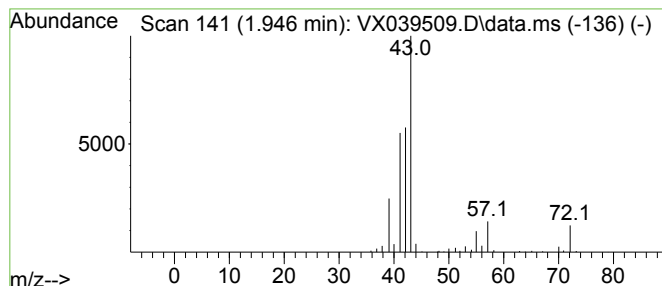
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Quant Title : SW846 8260

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

Peak Number 4 Pentane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.946	16.22 ug/l	99429	Pentafluorobenzene	5.549

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	86
2			Tetrahydrofuran	72	C4H8O	000109-99-9	47
3			Oxirane, ethyl-	72	C4H8O	000106-88-7	42
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
5			Pentane, 1-chloro-	106	C5H11Cl	000543-59-9	28



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122823\
Data File : VX039509.D
Acq On : 28 Dec 2023 12:29
Operator : JC/MD
Sample : 06024-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1222

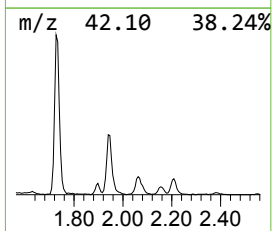
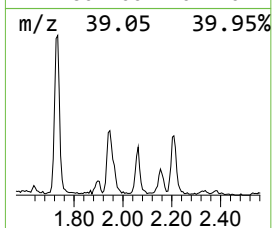
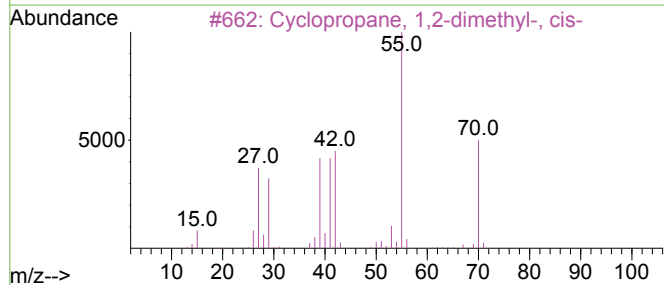
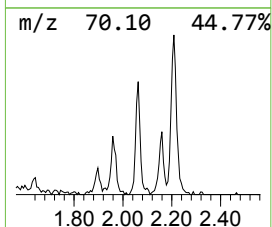
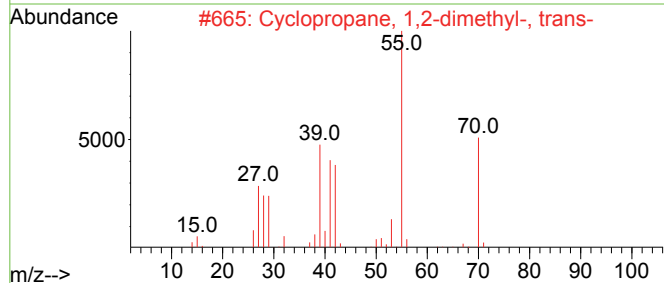
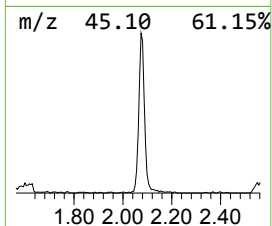
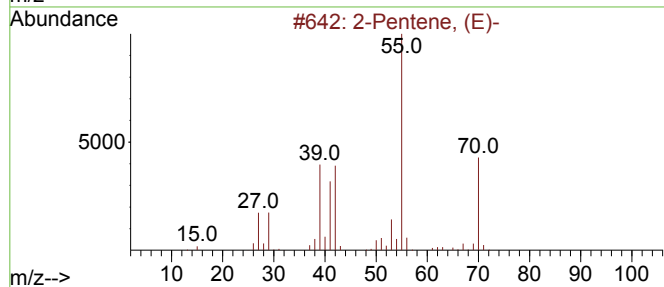
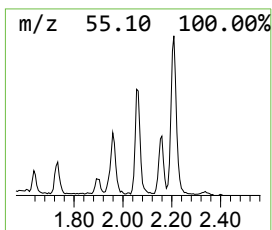
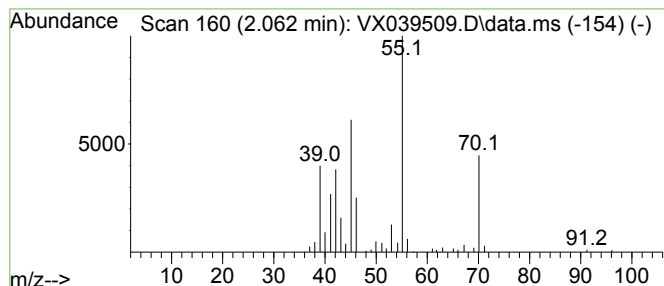
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Quant Title : SW846 8260

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

Peak Number 5 2-Pentene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.062	13.04 ug/l	79936	Pentafluorobenzene	5.549

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentene, (E)-	70	C5H10	000646-04-8	70
2			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	62
3			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	52
4			2-Pentene, (Z)-	70	C5H10	000627-20-3	50
5			2-Butene, 2-methyl-	70	C5H10	000513-35-9	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122823\
Data File : VX039509.D
Acq On : 28 Dec 2023 12:29
Operator : JC/MD
Sample : 06024-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1222

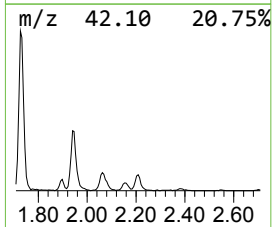
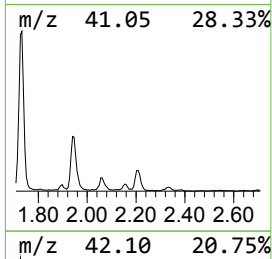
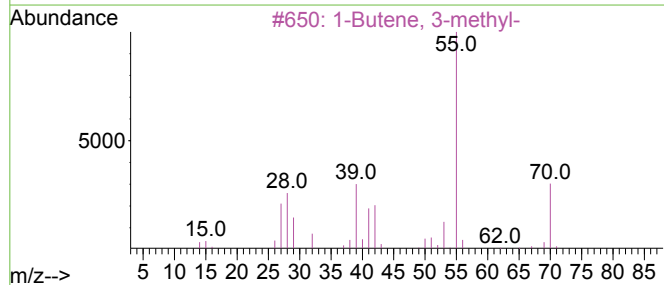
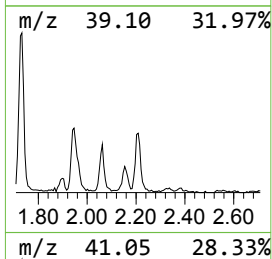
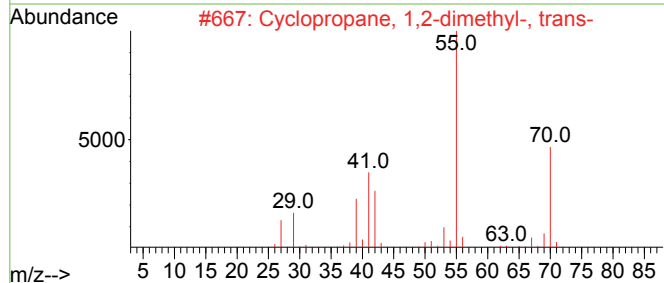
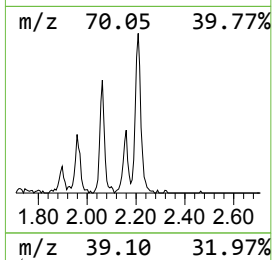
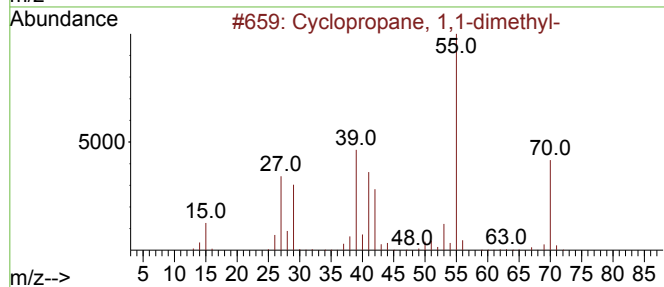
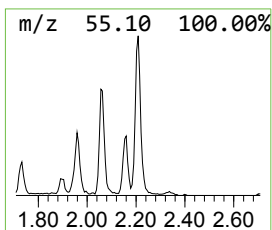
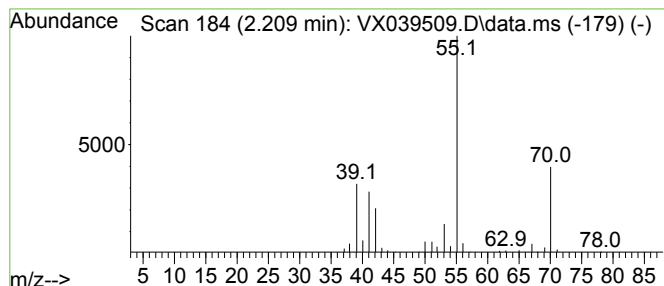
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Quant Title : SW846 8260

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

Peak Number 6 Cyclopropane, 1,1-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.209	10.37 ug/l	63547	Pentafluorobenzene	5.549

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	90
2			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	87
3			1-Butene, 3-methyl-	70	C5H10	000563-45-1	86
4			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	64
5			2-Butene, 2-methyl-	70	C5H10	000513-35-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122823\
Data File : VX039509.D
Acq On : 28 Dec 2023 12:29
Operator : JC/MD
Sample : 06024-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1222

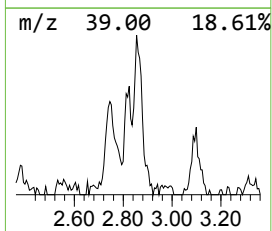
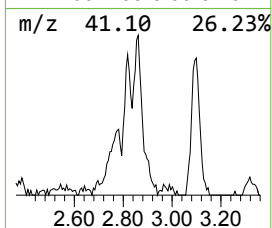
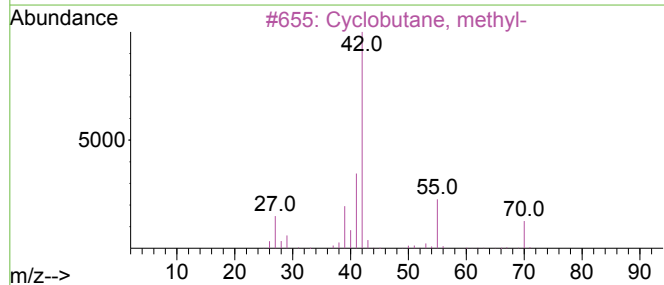
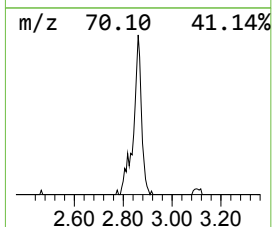
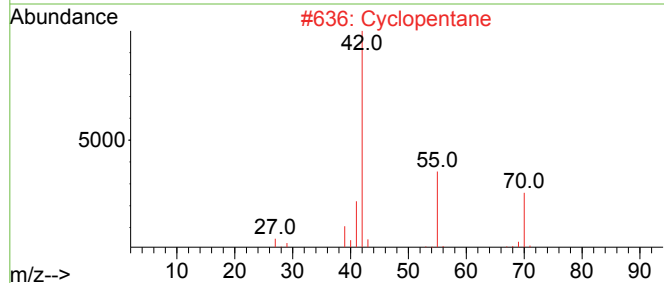
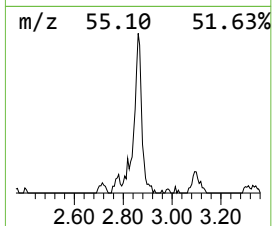
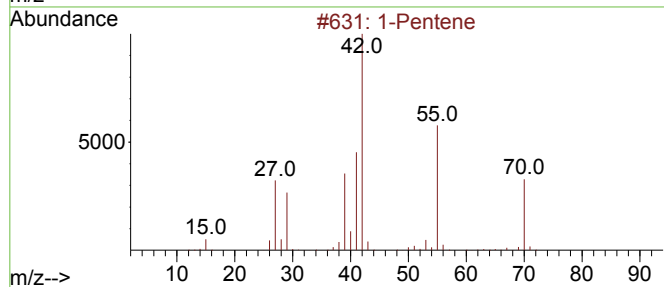
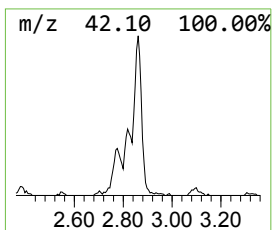
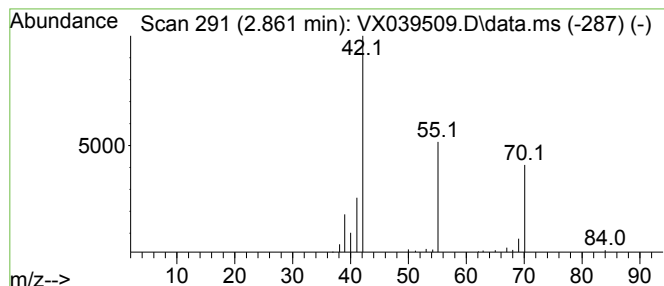
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Quant Title : SW846 8260

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

Peak Number 7 1-Pentene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.861	6.41 ug/l	39279	Pentafluorobenzene	5.549

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene			70	C5H10	000109-67-1	78
2	Cyclopentane			70	C5H10	000287-92-3	78
3	Cyclobutane, methyl-			70	C5H10	000598-61-8	72
4	1-Pentanol			88	C5H12O	000071-41-0	40
5	2-Pentene			70	C5H10	000109-68-2	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122823\
Data File : VX039509.D
Acq On : 28 Dec 2023 12:29
Operator : JC/MD
Sample : 06024-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1222

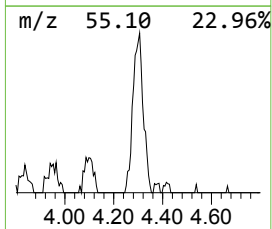
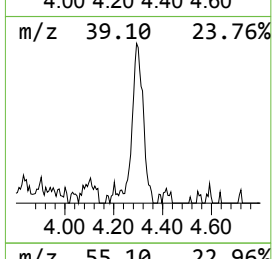
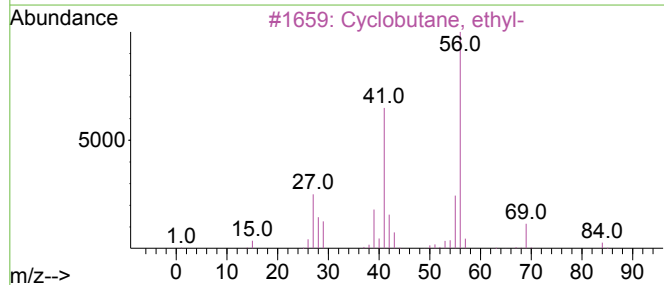
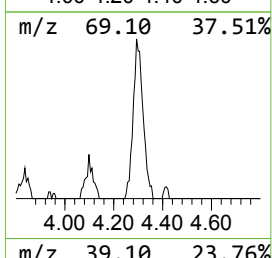
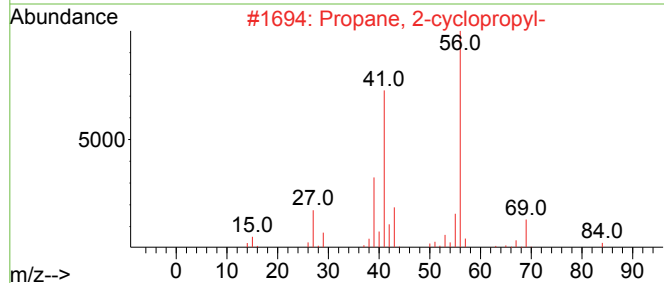
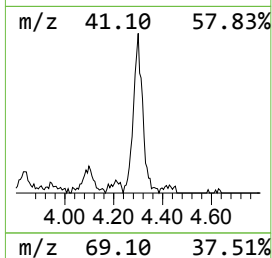
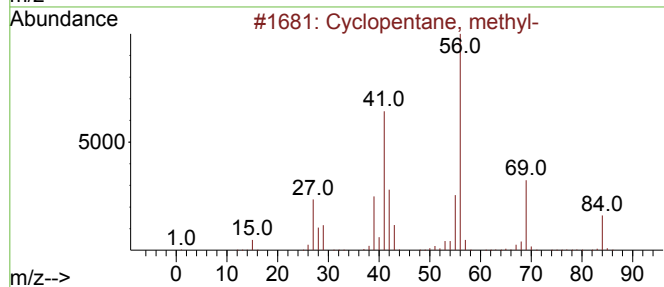
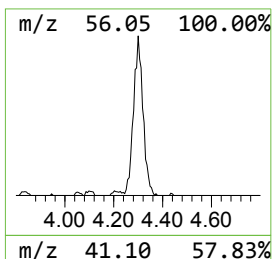
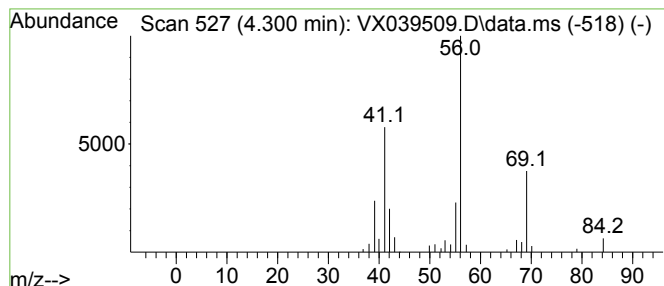
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Quant Title : SW846 8260

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

Peak Number 8 Cyclopentane, methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.300	7.65 ug/l	46865	Pentafluorobenzene	5.549

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	83
2			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	72
3			Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
4			Cyclopropane, propyl-	84	C6H12	002415-72-7	64
5			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122823\
Data File : VX039509.D
Acq On : 28 Dec 2023 12:29
Operator : JC/MD
Sample : 06024-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1222

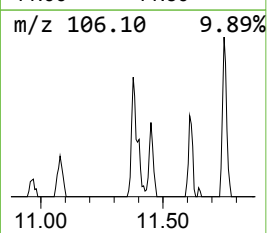
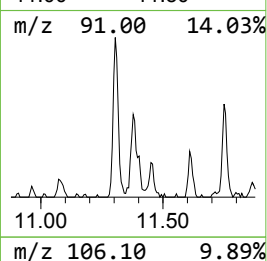
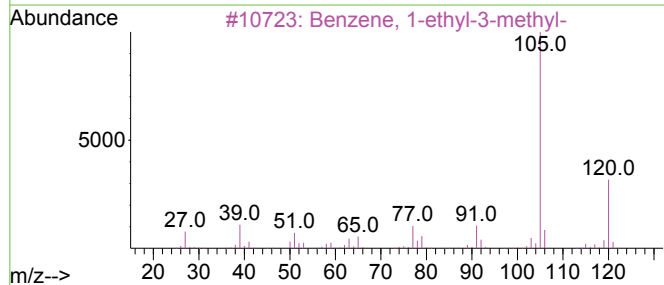
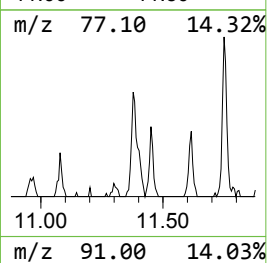
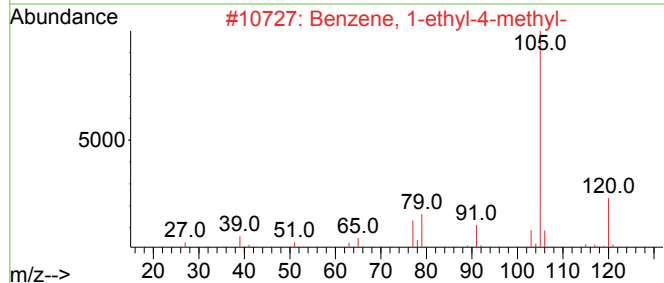
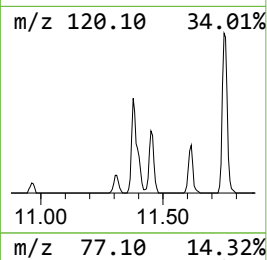
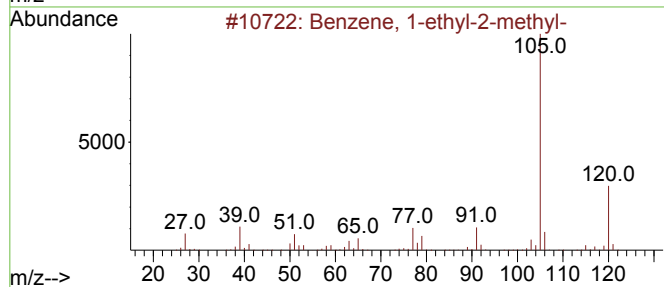
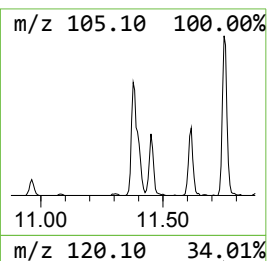
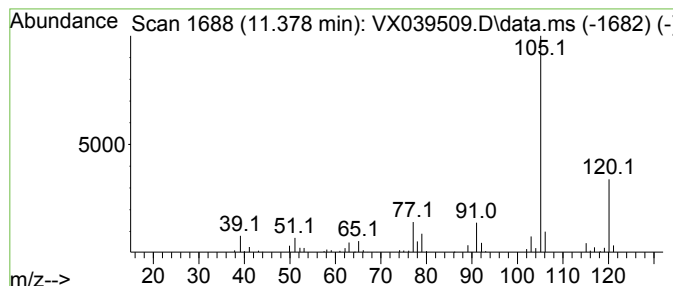
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	5.87 ug/l	60535	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122823\
Data File : VX039509.D
Acq On : 28 Dec 2023 12:29
Operator : JC/MD
Sample : 06024-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1222

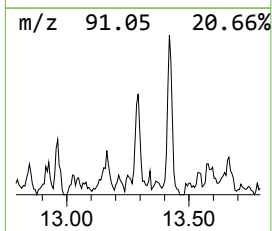
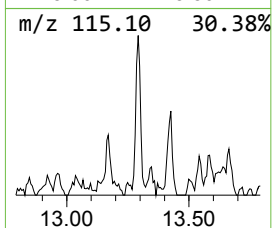
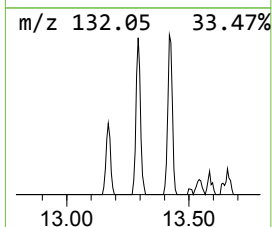
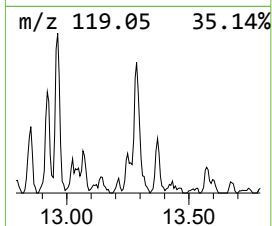
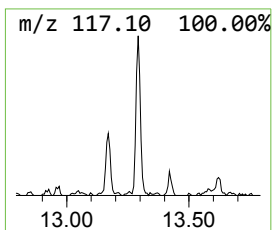
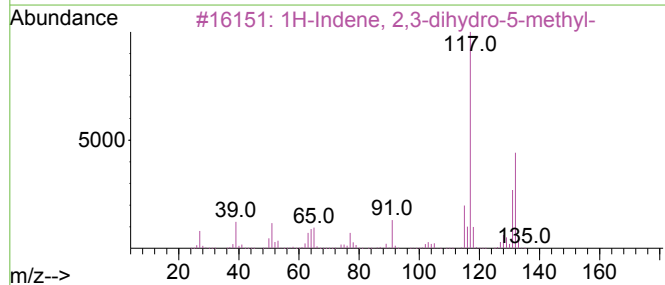
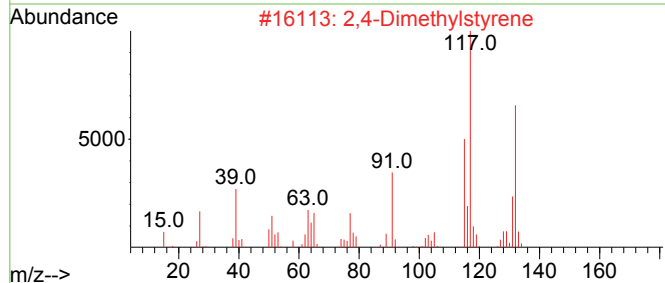
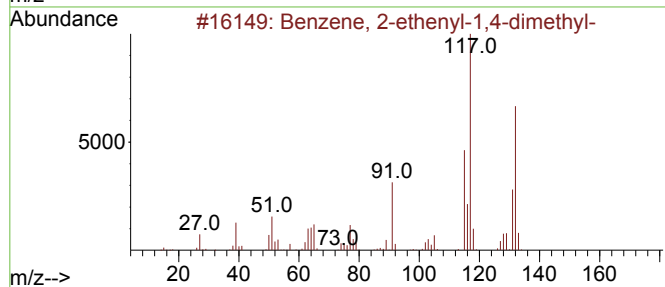
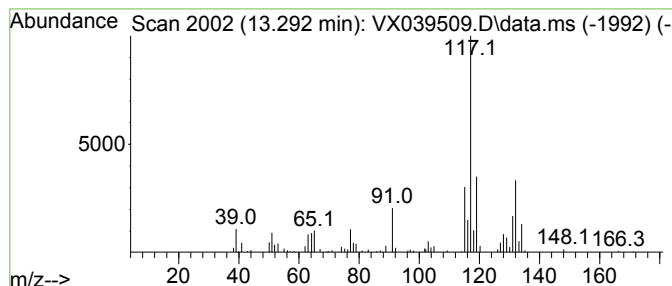
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	5.84 ug/l	60240	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2			2,4-Dimethylstyrene	132	C10H12	002234-20-0	92
3			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
4			Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	87
5			3-Phenylbut-1-ene	132	C10H12	000934-10-1	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122823\
Data File : VX039509.D
Acq On : 28 Dec 2023 12:29
Operator : JC/MD
Sample : 06024-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1222

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.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
Isobutane	1.264	8.4	ug/l	51616	1	5.549	306489	50.0
Butane	1.367	50.9	ug/l	312126	1	5.549	306489	50.0
Butane, 2-methyl-	1.727	34.3	ug/l	209953	1	5.549	306489	50.0
Pentane	1.946	16.2	ug/l	99429	1	5.549	306489	50.0
2-Pentene, (E)-	2.062	13.0	ug/l	79936	1	5.549	306489	50.0
Cyclopropane, 1...	2.209	10.4	ug/l	63547	1	5.549	306489	50.0
1-Pentene	2.861	6.4	ug/l	39279	1	5.549	306489	50.0
Cyclopentane, m...	4.300	7.7	ug/l	46865	1	5.549	306489	50.0
Benzene, 1-ethy...	11.378	5.9	ug/l	60535	4	12.024	515846	50.0
Benzene, 2-ethe...	13.292	5.8	ug/l	60240	4	12.024	515846	50.0