

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040824\
 Data File : VX040937.D
 Acq On : 08 Apr 2024 18:03
 Operator : JC/MD
 Sample : P2026-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 50312

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\82X040124W.M
 Title : SW846 8260

Signal : TIC: VX040937.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.270	27	30	41	rBV	21829	23519	2.36%	0.479%
2	1.374	41	47	53	rVV	202688	198365	19.91%	4.040%
3	1.429	53	56	57	rVV	16513	14528	1.46%	0.296%
4	1.453	57	60	65	rVV	141761	153775	15.43%	3.132%
5	1.496	65	67	76	rVB	15731	18271	1.83%	0.372%
6	1.752	104	109	119	rVB	55275	74172	7.44%	1.511%
7	1.959	139	143	152	rVB3	26748	50450	5.06%	1.027%
8	2.050	152	158	173	rVV	265206	485143	48.69%	9.880%
9	2.166	173	177	181	rVV	11256	16918	1.70%	0.345%
10	2.215	181	185	194	rVB	33035	50460	5.06%	1.028%
11	2.752	266	273	282	rBV2	9565	20270	2.03%	0.413%
12	2.867	288	292	303	rVB	8682	17837	1.79%	0.363%
13	3.111	324	332	343	rBB2	13688	32544	3.27%	0.663%
14	3.764	429	439	447	rBV5	5796	16624	1.67%	0.339%
15	4.300	517	527	538	rBB5	4958	14610	1.47%	0.298%
16	4.715	586	595	610	rBV	26994	75836	7.61%	1.544%
17	5.385	693	705	714	rBV3	28610	82954	8.33%	1.689%
18	5.550	724	732	747	rVB	44473	123590	12.40%	2.517%
19	5.958	790	799	804	rBV	32908	86576	8.69%	1.763%
20	6.038	804	812	828	rVB	223754	590805	59.29%	12.032%
21	6.763	921	931	943	rBV	72759	175589	17.62%	3.576%
22	8.647	1234	1240	1246	rBV	154489	243291	24.42%	4.955%
23	8.720	1246	1252	1266	rVB	624374	996399	100.00%	20.292%
24	10.055	1465	1471	1489	rVB	168769	234781	23.56%	4.781%
25	10.195	1489	1494	1502	rBV	44577	59841	6.01%	1.219%
26	10.299	1505	1511	1526	rVB	152800	202588	20.33%	4.126%
27	10.640	1562	1567	1577	rVB	75780	100875	10.12%	2.054%
28	11.079	1634	1639	1651	rBB	149136	191251	19.19%	3.895%
29	11.378	1684	1688	1696	rBV	19608	33168	3.33%	0.675%
30	11.451	1696	1700	1704	rVB	10753	12410	1.25%	0.253%
31	11.610	1722	1726	1735	rBV	9031	11960	1.20%	0.244%
32	11.750	1744	1749	1757	rVB	34476	43179	4.33%	0.879%
33	12.018	1788	1793	1800	rBV	202973	256649	25.76%	5.227%
34	12.085	1800	1804	1810	rVB	16779	19913	2.00%	0.406%
35	12.244	1823	1830	1838	rBV2	12002	19174	1.92%	0.390%
36	13.292	1997	2002	2007	rVB2	16752	22900	2.30%	0.466%

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Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040124W.M

Title : SW846 8260

37	13.420	2019	2023	2030	rVB	9867	12581	1.26%	0.256%
38	13.774	2074	2081	2089	rVB	7092	10579	1.06%	0.215%
39	13.926	2099	2106	2110	rBV2	6992	10662	1.07%	0.217%
40	14.225	2149	2155	2160	rBV3	16142	29979	3.01%	0.611%
41	14.371	2174	2179	2183	rVB2	8500	10589	1.06%	0.216%
42	14.481	2192	2197	2202	rBV2	13734	17588	1.77%	0.358%
43	14.615	2214	2219	2221	rBV2	9752	13572	1.36%	0.276%
44	15.182	2307	2312	2320	rVB	11772	21677	2.18%	0.441%
45	15.487	2357	2362	2365	rBV4	7182	11835	1.19%	0.241%

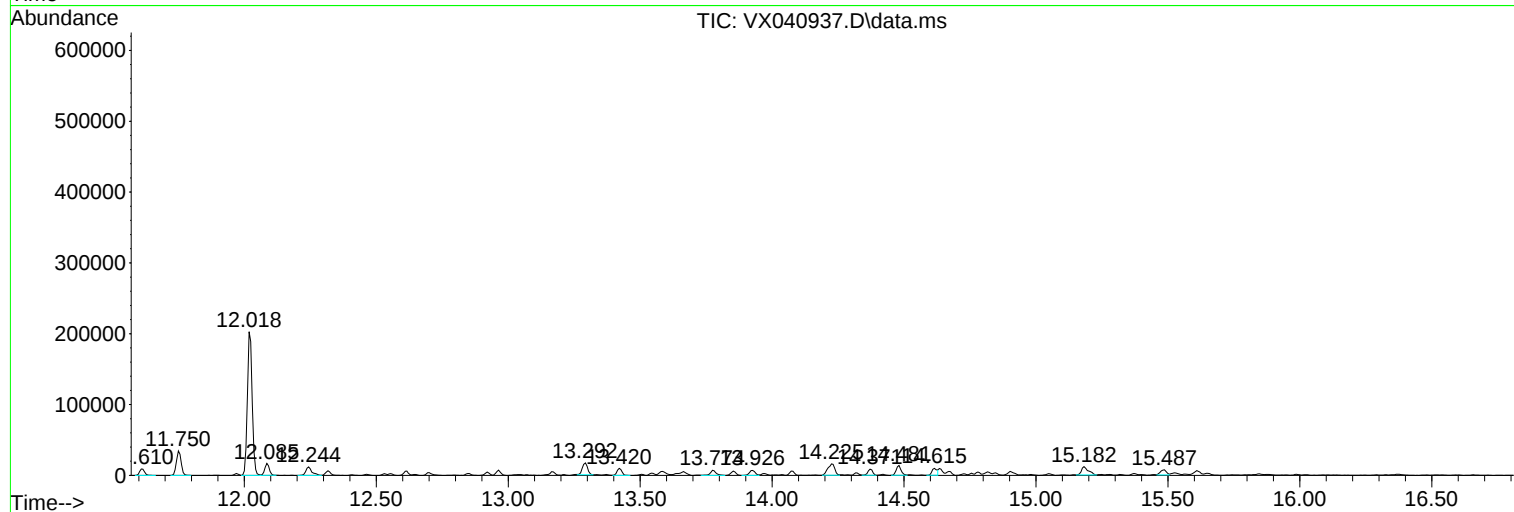
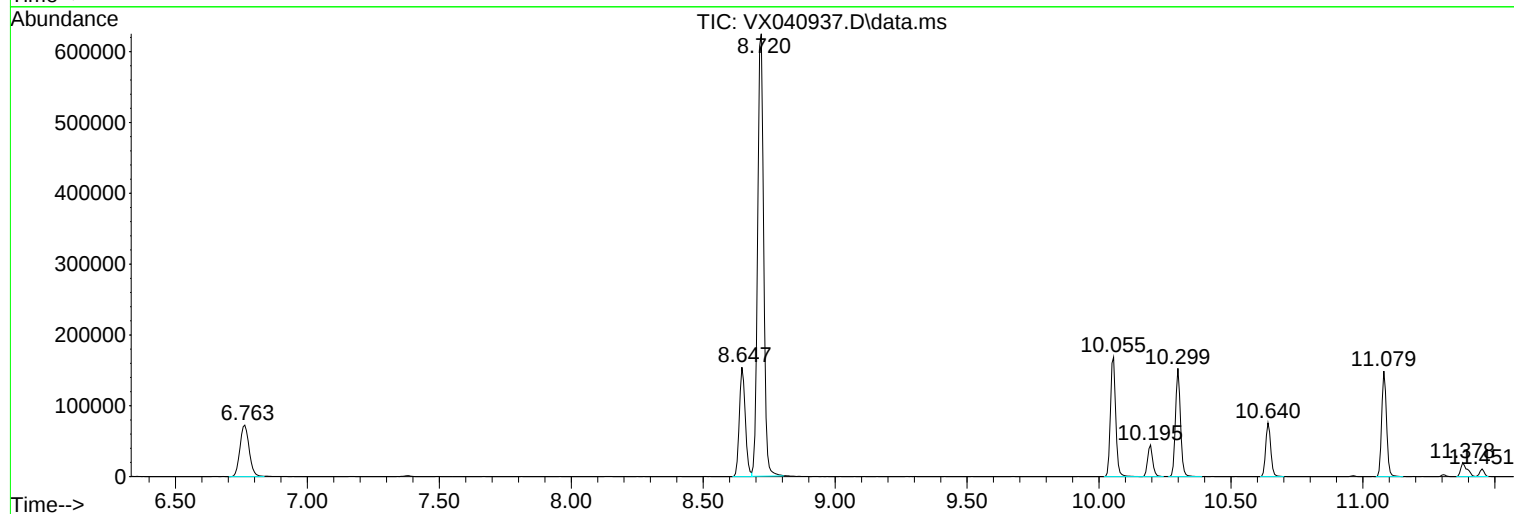
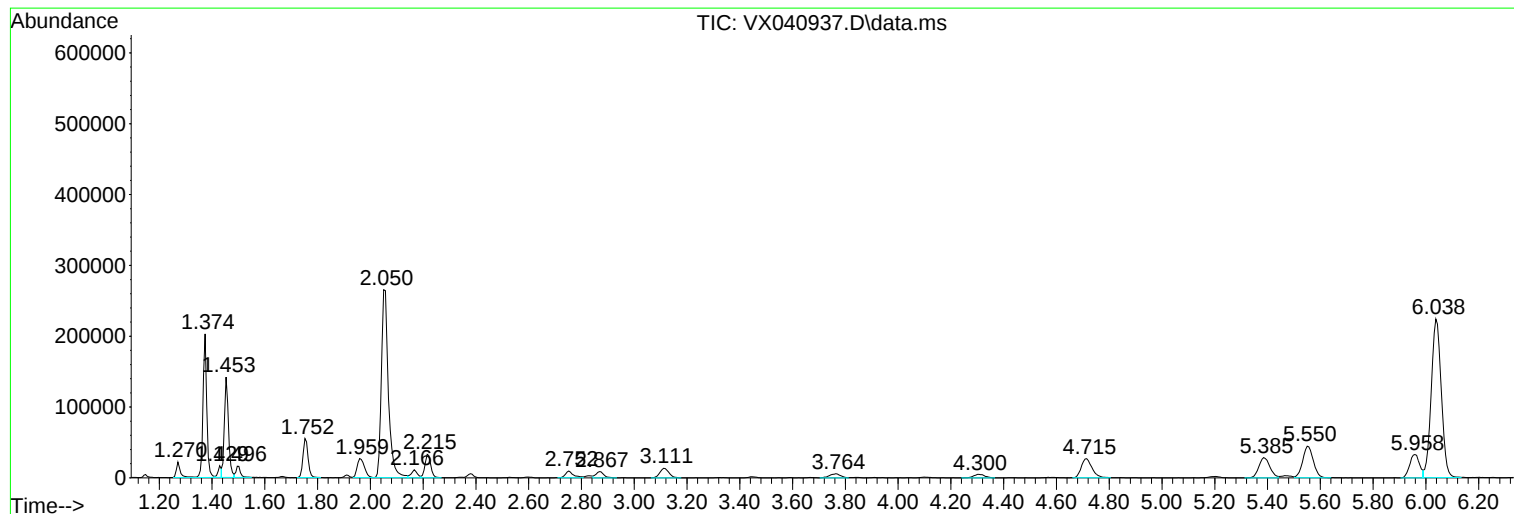
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040124W.M
Quant Title : SW846 8260

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



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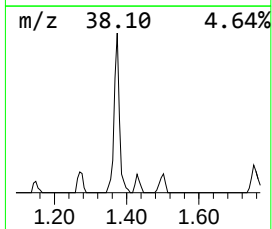
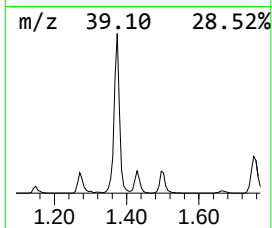
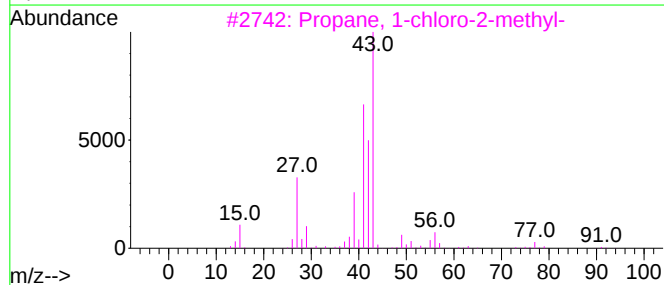
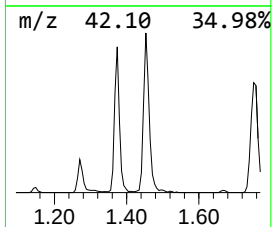
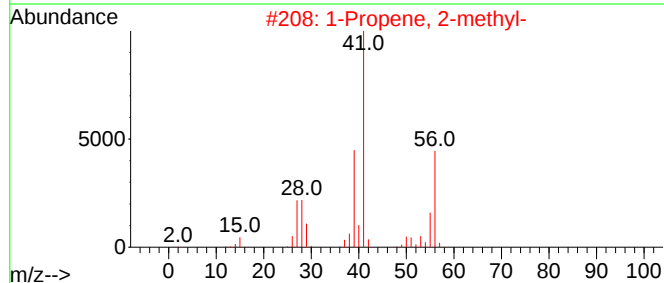
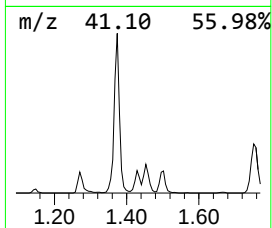
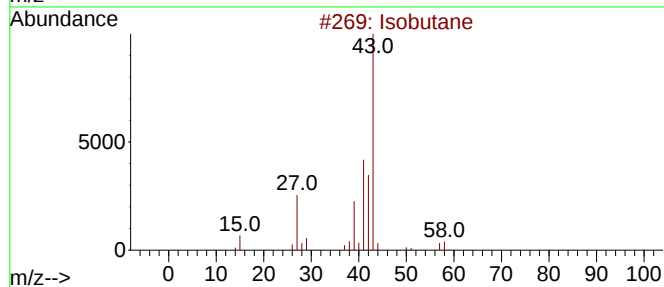
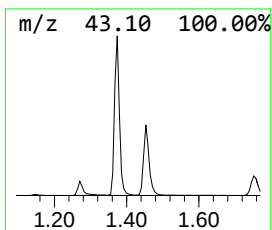
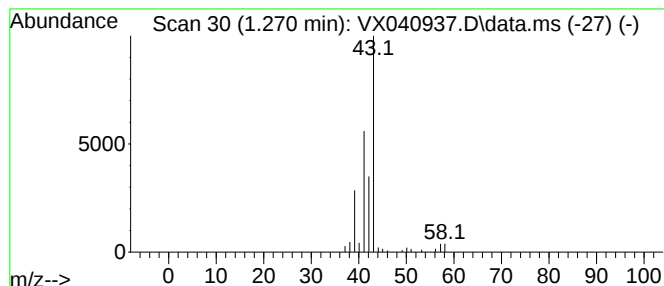
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Quant Title : SW846 8260

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

Peak Number 1 Isobutane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.270	9.51 ug/l	23519	Pentafluorobenzene	5.550

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isobutane	58	C4H10	000075-28-5	64
2		1-Propene, 2-methyl-	56	C4H8	000115-11-7	9
3		Propane, 1-chloro-2-methyl-	92	C4H9Cl	000513-36-0	9
4		Borane, trimethyl-	56	C3H9B	000593-90-8	5
5		Propene	42	C3H6	000115-07-1	5



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50312

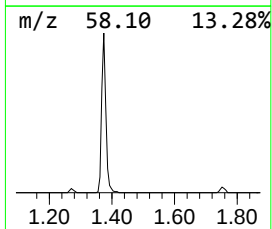
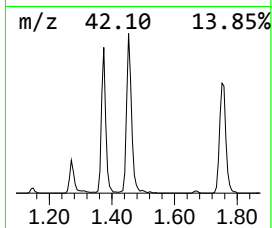
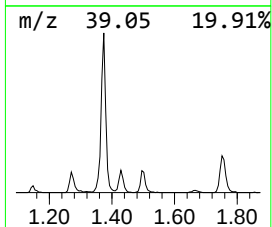
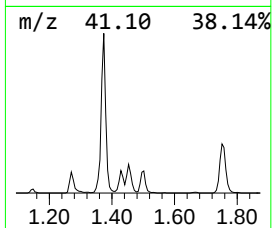
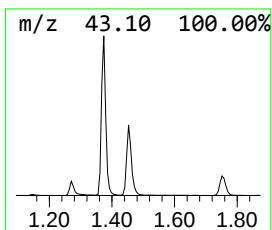
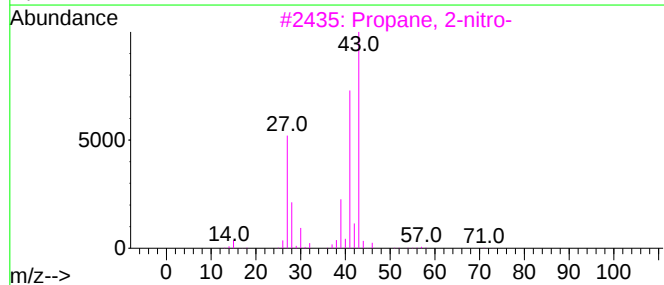
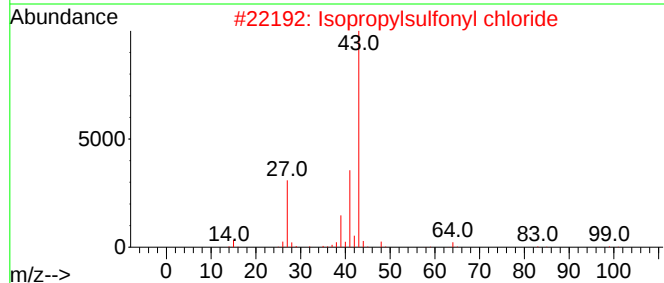
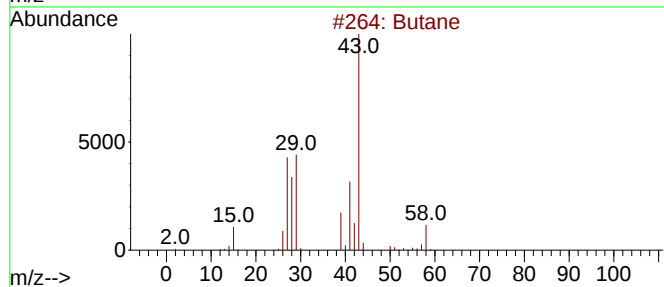
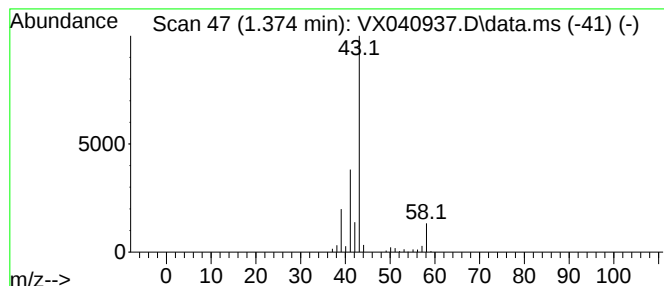
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040124W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.374	80.25 ug/l	198365	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	72
2			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
3			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	9
4			Isobutane	58	C4H10	000075-28-5	9
5			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040824\
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Sample : P2026-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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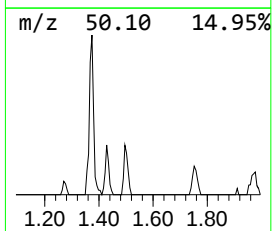
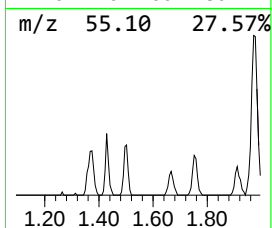
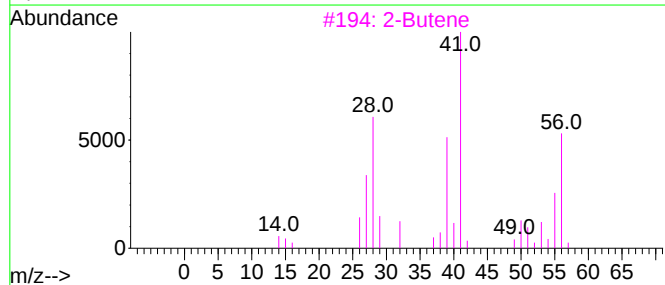
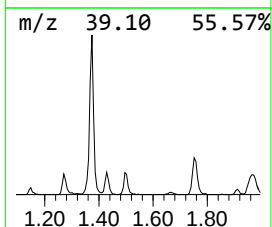
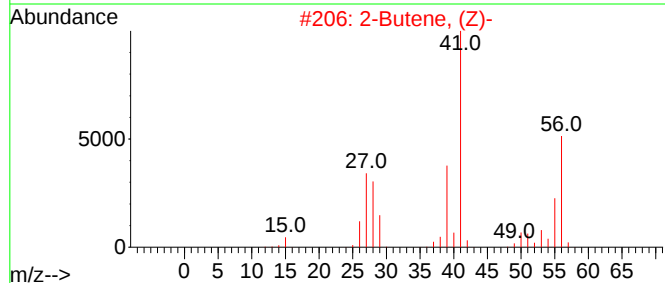
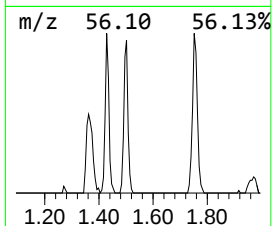
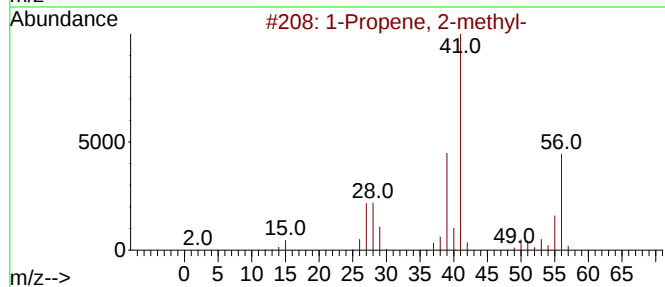
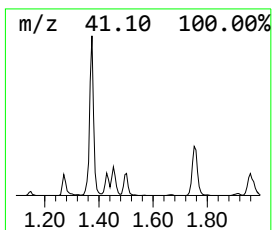
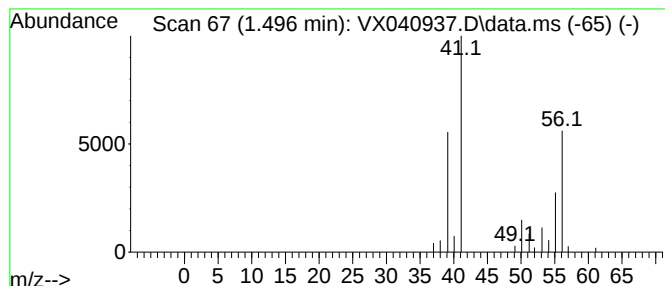
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040124W.M
Quant Title : SW846 8260

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

Peak Number 4 1-Propene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.496	7.39 ug/l	18271	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methyl-			56	C4H8	000115-11-7	87
2	2-Butene, (Z)-			56	C4H8	000590-18-1	72
3	2-Butene			56	C4H8	000107-01-7	64
4	1-Butene			56	C4H8	000106-98-9	52
5	Cyclobutane			56	C4H8	000287-23-0	47



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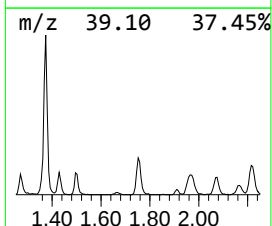
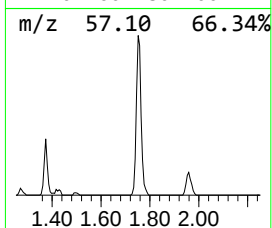
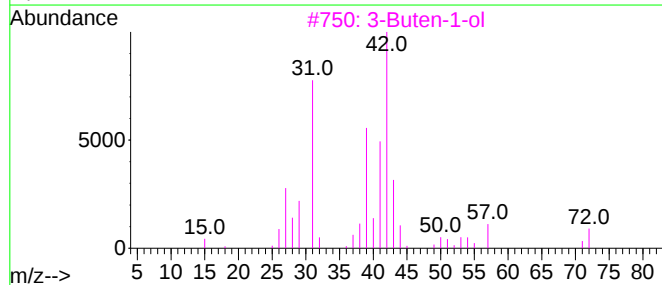
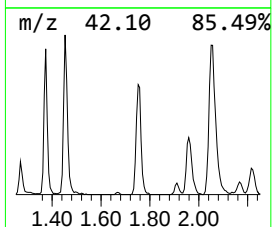
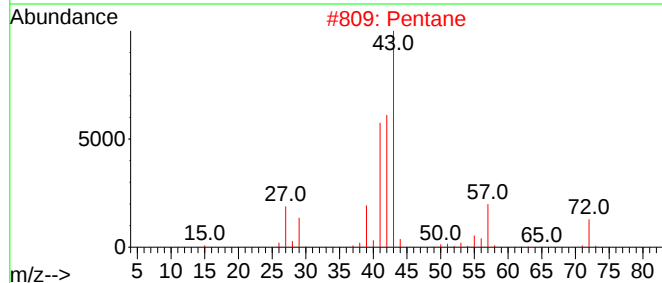
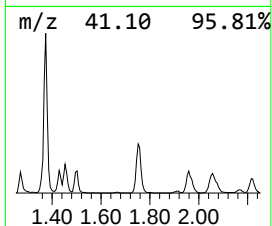
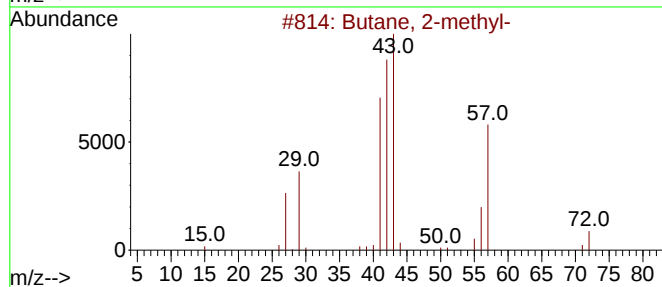
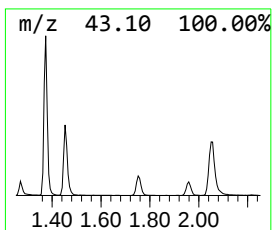
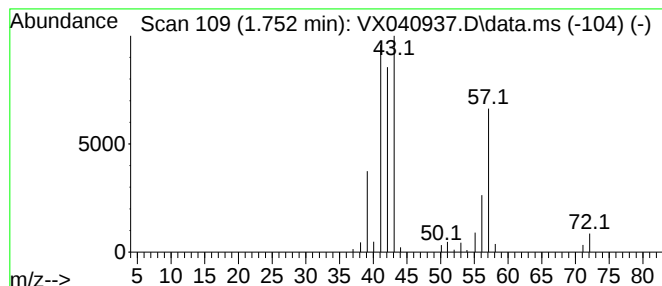
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Quant Title : SW846 8260

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

Peak Number 5 Butane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	30.01 ug/l	74172	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	86
2			Pentane	72	C5H12	000109-66-0	33
3			3-Buten-1-ol	72	C4H8O	000627-27-0	25
4			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	25
5			1-Propene, 2-methyl-	56	C4H8	000115-11-7	9



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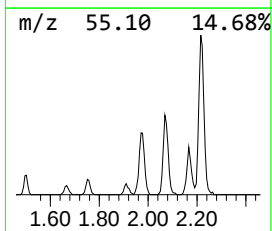
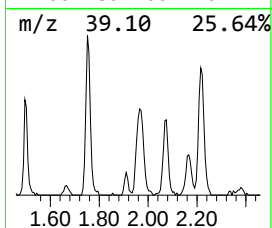
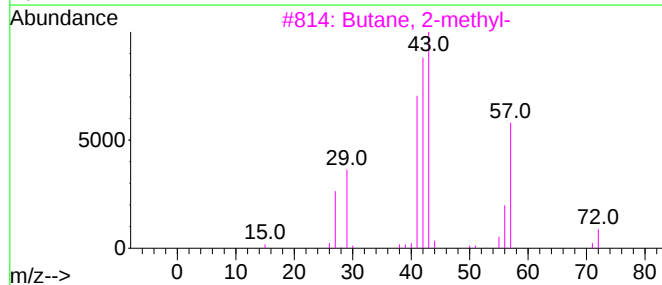
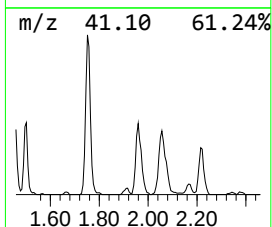
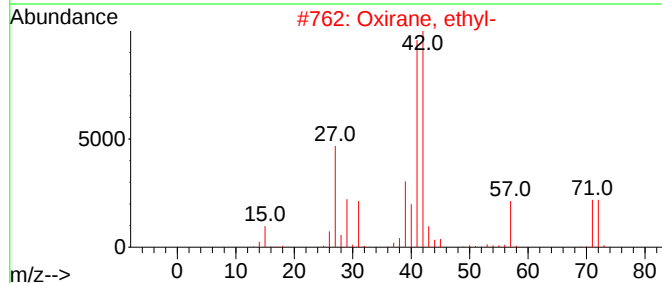
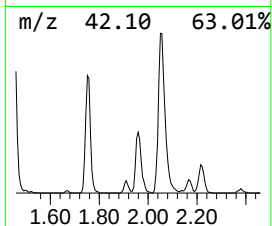
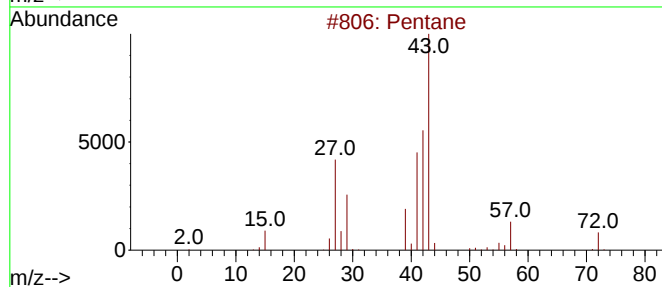
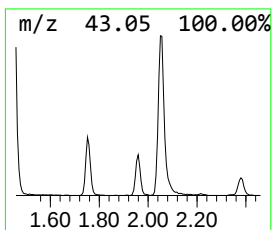
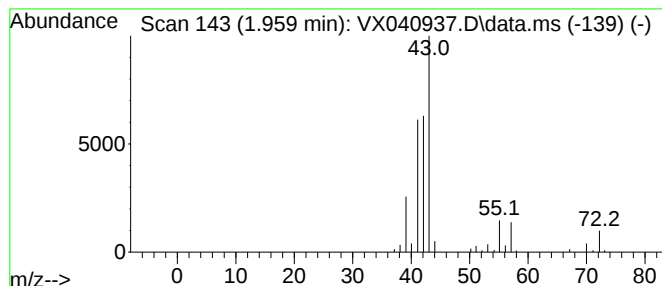
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Quant Title : SW846 8260

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

Peak Number 6 Pentane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.959	20.41 ug/l	50450	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	80
2			Oxirane, ethyl-	72	C4H8O	000106-88-7	50
3			Butane, 2-methyl-	72	C5H12	000078-78-4	45
4			Isobutyl nitrite	103	C4H9NO2	000542-56-3	17
5			Isobutylene epoxide	72	C4H8O	000558-30-5	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040824\
Data File : VX040937.D
Acq On : 08 Apr 2024 18:03
Operator : JC/MD
Sample : P2026-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50312

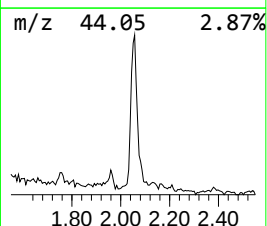
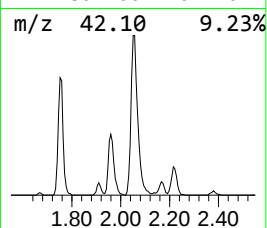
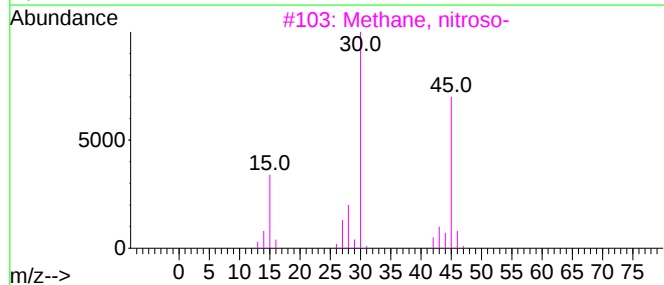
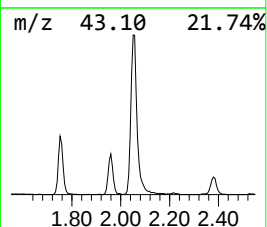
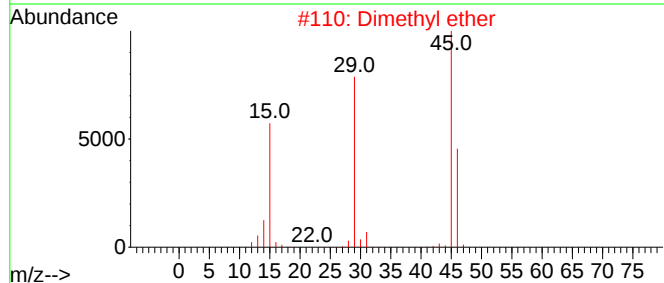
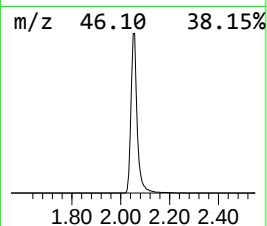
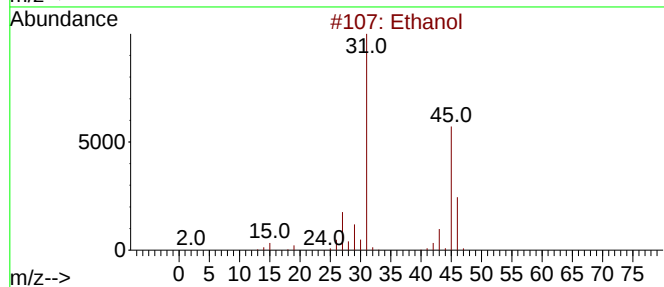
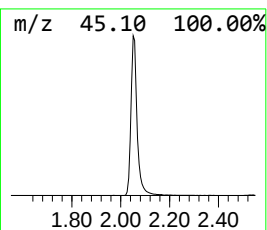
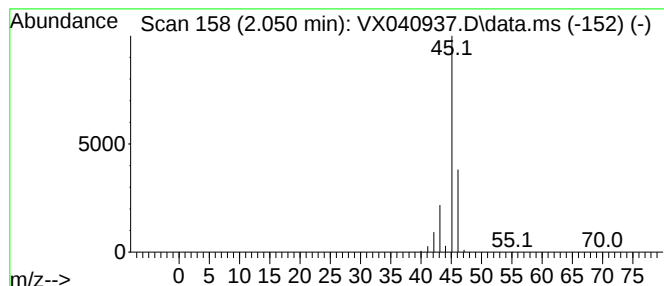
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Quant Title : SW846 8260

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

Peak Number 7 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.050	196.27 ug/l	485143	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	74
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Methane, nitroso-	45	CH3NO	000865-40-7	4
4			Formic acid	46	CH2O2	000064-18-6	4
5			L-Lactic acid	90	C3H6O3	000079-33-4	2



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040824\
Data File : VX040937.D
Acq On : 08 Apr 2024 18:03
Operator : JC/MD
Sample : P2026-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50312

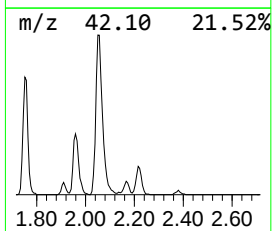
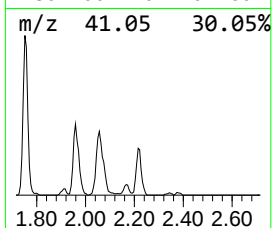
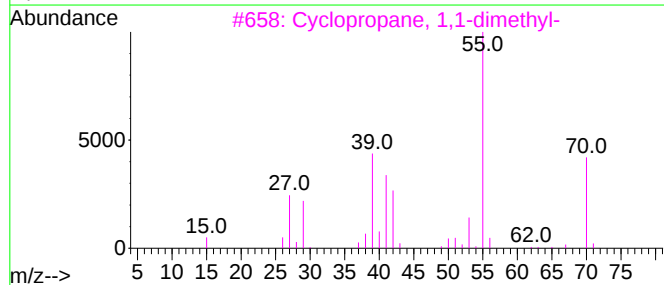
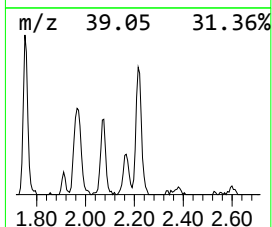
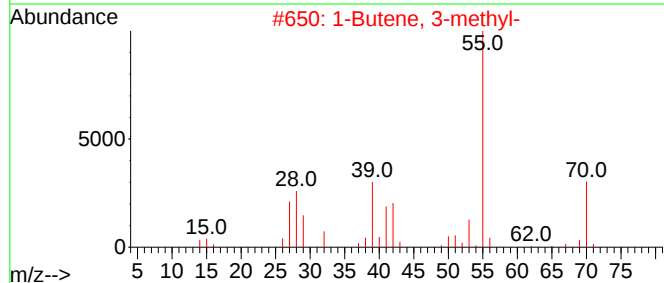
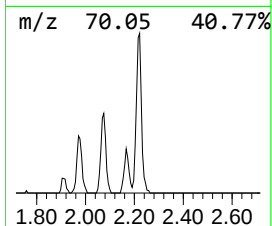
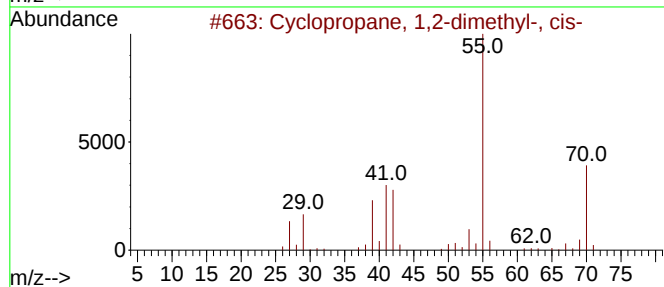
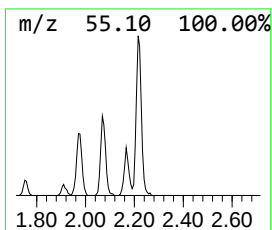
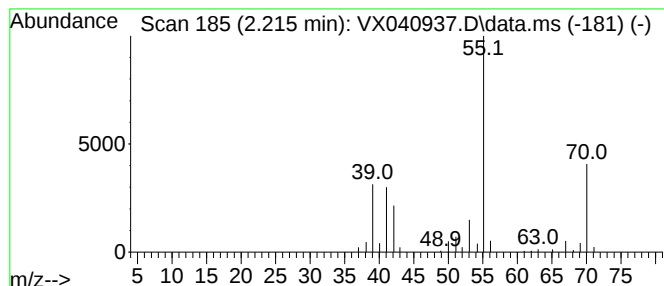
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Quant Title : SW846 8260

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

Peak Number 8 Cyclopropane, 1,2-dimethyl-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	20.41 ug/l	50460	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	90
2			1-Butene, 3-methyl-	70	C5H10	000563-45-1	86
3			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	83
4			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	80
5			2-Butene, 2-methyl-	70	C5H10	000513-35-9	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040824\
Data File : VX040937.D
Acq On : 08 Apr 2024 18:03
Operator : JC/MD
Sample : P2026-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50312

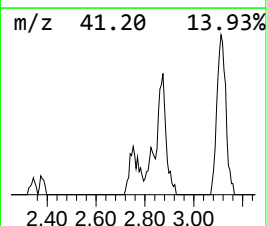
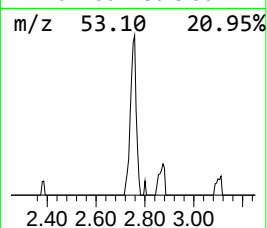
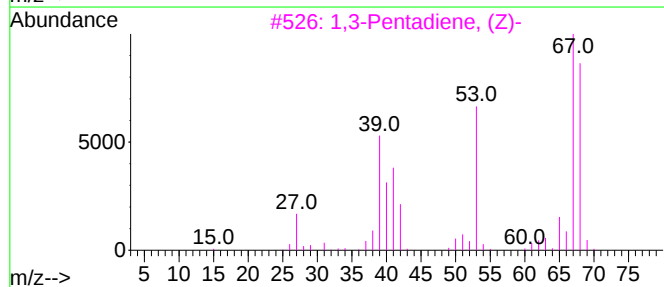
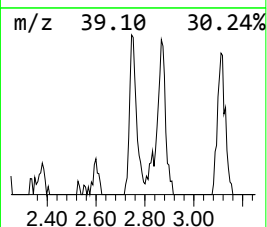
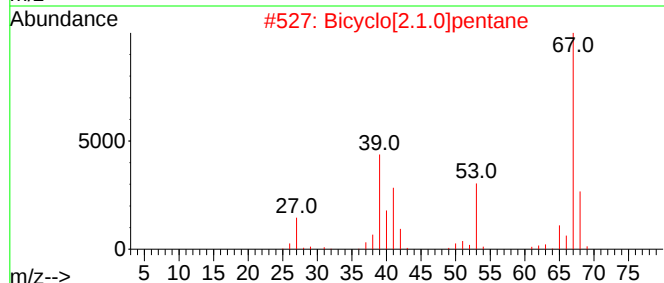
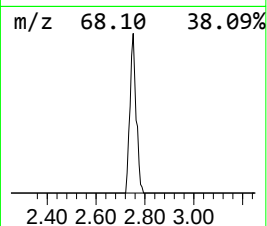
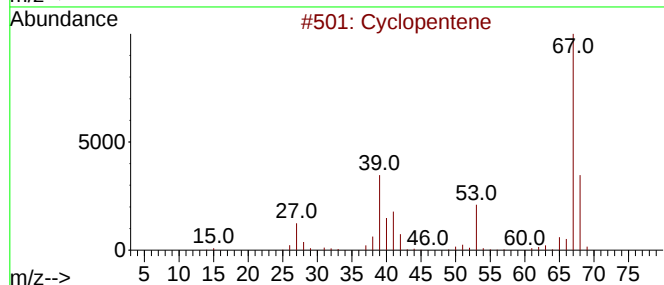
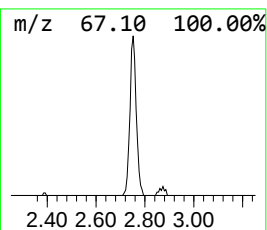
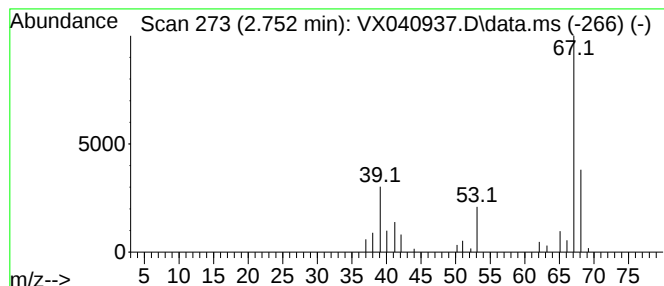
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Quant Title : SW846 8260

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

Peak Number 9 Cyclopentene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.752	8.20 ug/l	20270	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentene	68	C5H8	000142-29-0	91
2			Bicyclo[2.1.0]pentane	68	C5H8	000185-94-4	72
3			1,3-Pentadiene, (Z)-	68	C5H8	001574-41-0	58
4			1,3-Pentadiene, (E)-	68	C5H8	002004-70-8	58
5			1,3-Pentadiene	68	C5H8	000504-60-9	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040824\
Data File : VX040937.D
Acq On : 08 Apr 2024 18:03
Operator : JC/MD
Sample : P2026-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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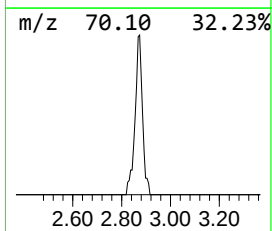
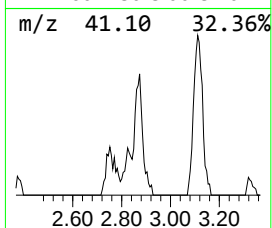
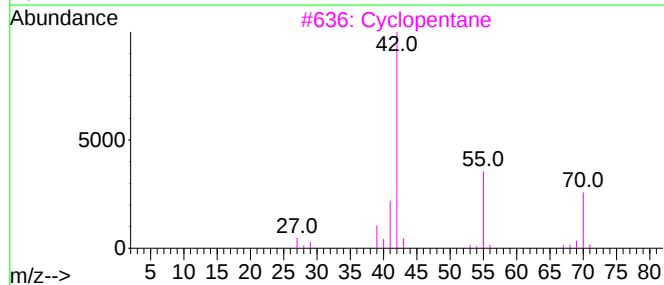
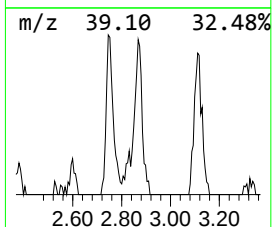
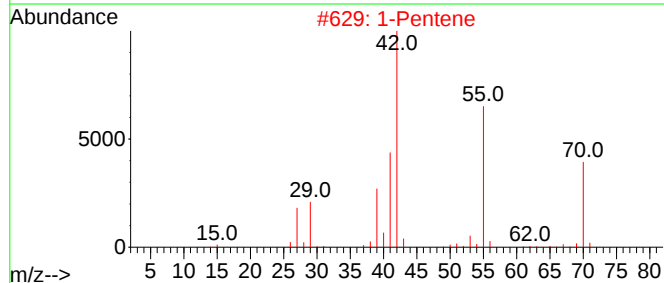
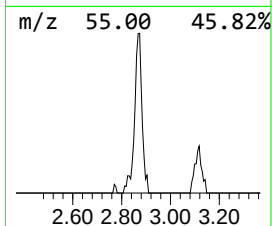
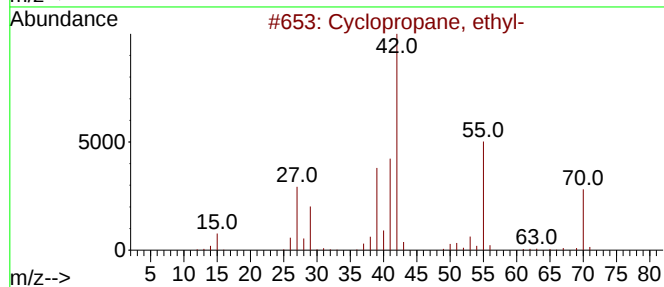
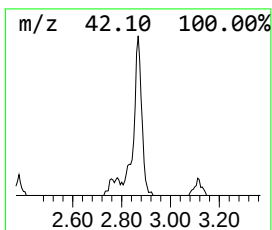
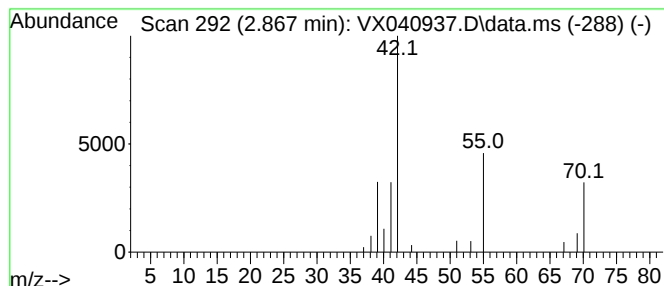
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Quant Title : SW846 8260

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

Peak Number 10 Cyclopropane, ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	7.22 ug/l	17837	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, ethyl-	70	C5H10	001191-96-4	80
2			1-Pentene	70	C5H10	000109-67-1	78
3			Cyclopentane	70	C5H10	000287-92-3	9
4			Cyclobutanone	70	C4H6O	001191-95-3	9
5			Cyclobutane, methyl-	70	C5H10	000598-61-8	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040824\
Data File : VX040937.D
Acq On : 08 Apr 2024 18:03
Operator : JC/MD
Sample : P2026-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50312

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040124W.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
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Butane	1.374	80.3	ug/l	198365	1	5.550	123590	50.0
1-Propene, 2-me...	1.496	7.4	ug/l	18271	1	5.550	123590	50.0
Butane, 2-methyl-	1.752	30.0	ug/l	74172	1	5.550	123590	50.0
Pentane	1.959	20.4	ug/l	50450	1	5.550	123590	50.0
Ethanol	2.050	196.3	ug/l	485143	1	5.550	123590	50.0
Cyclopropane, 1...	2.215	20.4	ug/l	50460	1	5.550	123590	50.0
Cyclopentene	2.752	8.2	ug/l	20270	1	5.550	123590	50.0
Cyclopropane, e...	2.867	7.2	ug/l	17837	1	5.550	123590	50.0