

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040824\
 Data File : VX040934.D
 Acq On : 08 Apr 2024 16:54
 Operator : JC/MD
 Sample : P2026-04 40X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 50313

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: VX040934.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	25	30	38	rBV	11399	11939	3.34%	0.359%
2	1.374	42	47	53	rVV	98643	96983	27.10%	2.917%
3	1.429	53	56	58	rVV	9403	9132	2.55%	0.275%
4	1.453	58	60	65	rVV	10445	11596	3.24%	0.349%
5	1.496	65	67	72	rVB	8808	8957	2.50%	0.269%
6	1.752	105	109	117	rVB	17580	23551	6.58%	0.708%
7	1.965	139	144	152	rVV2	9455	19746	5.52%	0.594%
8	2.050	152	158	173	rVV	200147	357913	100.00%	10.763%
9	2.166	173	177	181	rVV2	6069	10777	3.01%	0.324%
10	2.215	181	185	193	rVB	16977	26386	7.37%	0.793%
11	2.380	205	212	218	rBV2	2726	4802	1.34%	0.144%
12	2.752	267	273	278	rBV2	4186	7486	2.09%	0.225%
13	2.873	287	293	300	rVB2	3221	6606	1.85%	0.199%
14	3.111	326	332	341	rBV3	4955	11646	3.25%	0.350%
15	3.764	432	439	448	rVB4	1993	5115	1.43%	0.154%
16	4.715	585	595	613	rBV	33318	95350	26.64%	2.867%
17	5.385	695	705	716	rBV2	27713	80054	22.37%	2.407%
18	5.550	723	732	749	rVB	41138	116624	32.58%	3.507%
19	5.958	790	799	805	rBV	32292	86535	24.18%	2.602%
20	6.038	805	812	828	rVB	85168	226849	63.38%	6.822%
21	6.763	920	931	944	rBV	70549	168627	47.11%	5.071%
22	8.647	1234	1240	1246	rBV	147793	232102	64.85%	6.980%
23	8.720	1246	1252	1266	rVB	225469	355905	99.44%	10.703%
24	10.055	1465	1471	1480	rBV	162658	223563	62.46%	6.723%
25	10.195	1489	1494	1503	rVB	17641	22944	6.41%	0.690%
26	10.299	1506	1511	1518	rBV	59767	81318	22.72%	2.445%
27	10.640	1562	1567	1573	rBV	31061	40189	11.23%	1.209%
28	11.079	1634	1639	1651	rVB	146600	184419	51.53%	5.546%
29	11.305	1672	1676	1682	rVB	3543	4042	1.13%	0.122%
30	11.378	1684	1688	1695	rBV	14535	24808	6.93%	0.746%
31	11.451	1695	1700	1702	rVV2	7567	9824	2.74%	0.295%
32	11.476	1702	1704	1710	rVB	4664	5100	1.42%	0.153%
33	11.616	1722	1727	1733	rVB	8109	9917	2.77%	0.298%
34	11.750	1745	1749	1756	rVB	31188	37828	10.57%	1.138%
35	12.018	1788	1793	1800	rBV	191389	250947	70.11%	7.547%
36	12.085	1800	1804	1812	rVB	14618	19264	5.38%	0.579%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040824\
 Data File : VX040934.D
 Acq On : 08 Apr 2024 16:54
 Operator : JC/MD
 Sample : P2026-04 40X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 50313

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

37	12.244	1825	1830	1833	rBV	9067	13548	3.79%	0.407%
38	12.317	1838	1842	1850	rVB5	6112	10271	2.87%	0.309%
39	12.421	1853	1859	1863	rBV	8374	10737	3.00%	0.323%
40	12.463	1863	1866	1871	rVB	3493	4083	1.14%	0.123%
41	12.530	1873	1877	1879	rBV2	3399	4761	1.33%	0.143%
42	12.555	1879	1881	1886	rVB2	3694	3882	1.08%	0.117%
43	12.616	1886	1891	1894	rBV	3997	4531	1.27%	0.136%
44	12.695	1899	1904	1913	rVB3	4722	9198	2.57%	0.277%
45	12.963	1944	1948	1954	rVB2	6181	10073	2.81%	0.303%
46	13.164	1974	1981	1986	rBV4	6350	9201	2.57%	0.277%
47	13.268	1992	1998	1999	rBV	11605	14133	3.95%	0.425%
48	13.292	1999	2002	2006	rVB2	16210	22384	6.25%	0.673%
49	13.420	2019	2023	2033	rVB2	10012	14403	4.02%	0.433%
50	13.585	2046	2050	2054	rBV4	3571	5088	1.42%	0.153%
51	13.774	2077	2081	2087	rVB	17397	22794	6.37%	0.685%
52	13.847	2087	2093	2099	rVB3	5820	10049	2.81%	0.302%
53	13.920	2099	2105	2111	rVB8	4103	7079	1.98%	0.213%
54	14.036	2120	2124	2127	rBV	13625	14398	4.02%	0.433%
55	14.225	2150	2155	2162	rVB3	8330	15497	4.33%	0.466%
56	14.371	2176	2179	2182	rBV2	3572	4001	1.12%	0.120%
57	14.481	2192	2197	2208	rBV7	6354	12435	3.47%	0.374%
58	14.634	2215	2222	2227	rBV	32124	51259	14.32%	1.541%
59	14.756	2232	2242	2244	rBV	17841	25927	7.24%	0.780%
60	14.780	2244	2246	2251	rVV	20380	23785	6.65%	0.715%
61	14.963	2272	2276	2284	rVB5	2880	5200	1.45%	0.156%
62	15.176	2306	2311	2314	rBV5	4304	7500	2.10%	0.226%
63	15.207	2314	2316	2324	rVV2	8913	13670	3.82%	0.411%
64	15.274	2324	2327	2333	rVB5	2435	3913	1.09%	0.118%
65	15.371	2339	2343	2348	rBV4	4098	7086	1.98%	0.213%
66	15.487	2356	2362	2367	rBV2	20122	32372	9.04%	0.974%
67	15.609	2378	2382	2386	rBV	10905	17740	4.96%	0.533%
68	15.646	2386	2388	2393	rVB2	6215	8789	2.46%	0.264%
69	15.841	2412	2420	2424	rBV4	2930	6538	1.83%	0.197%
70	16.377	2499	2508	2514	rVB5	5239	10110	2.82%	0.304%

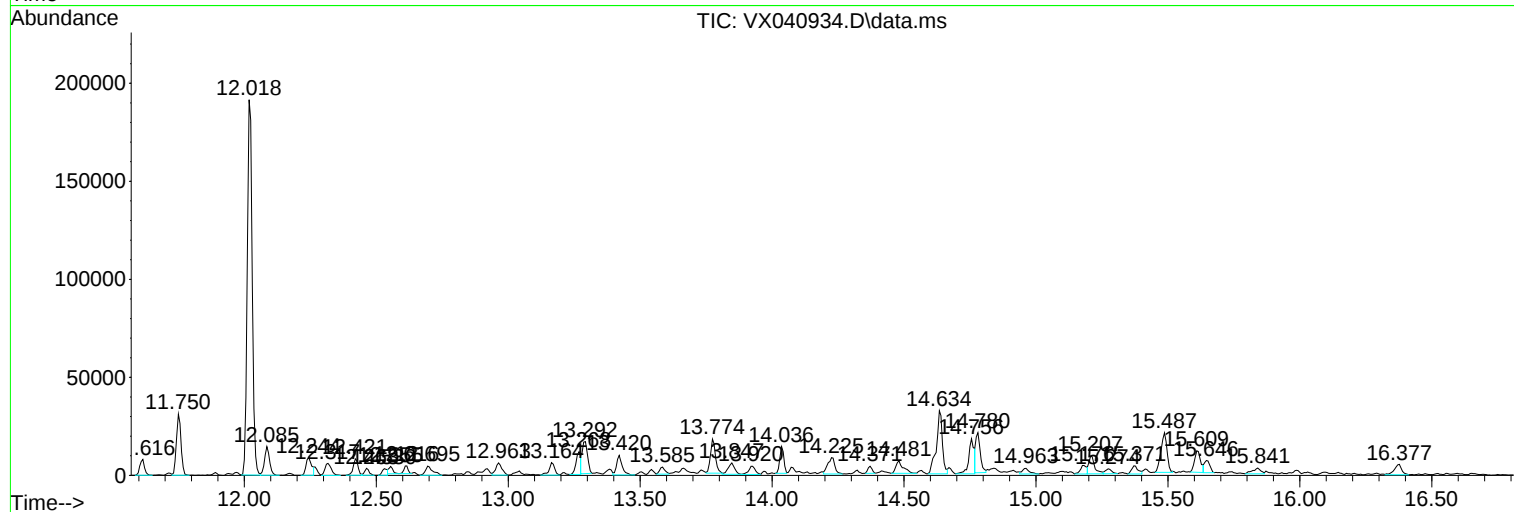
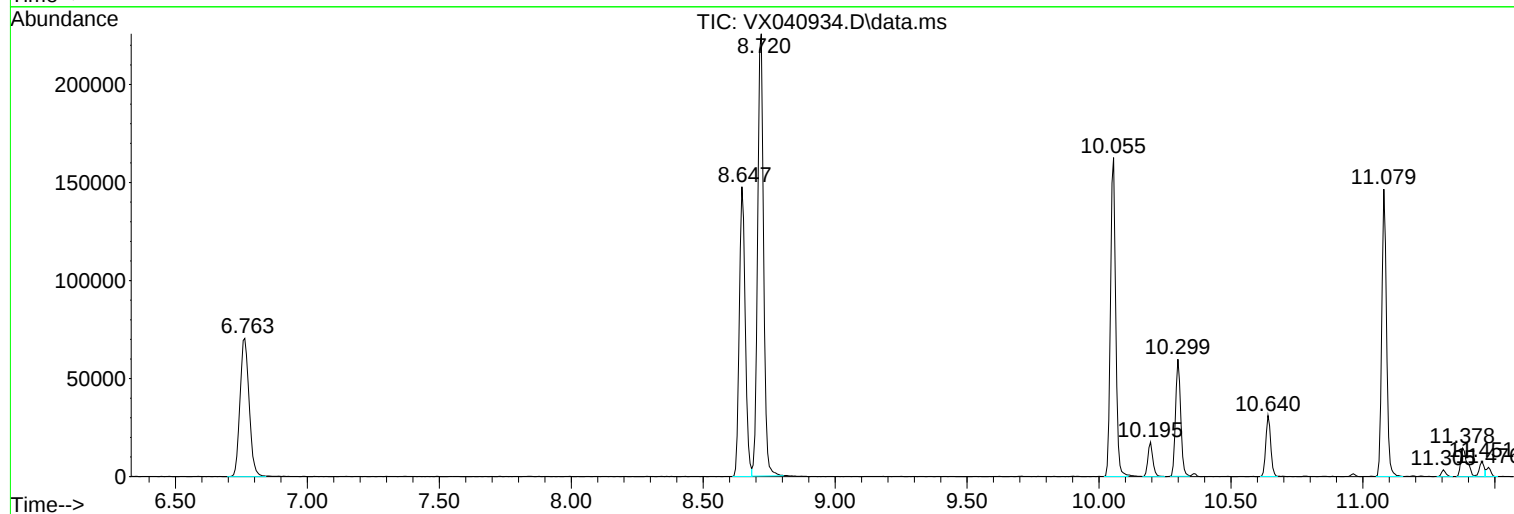
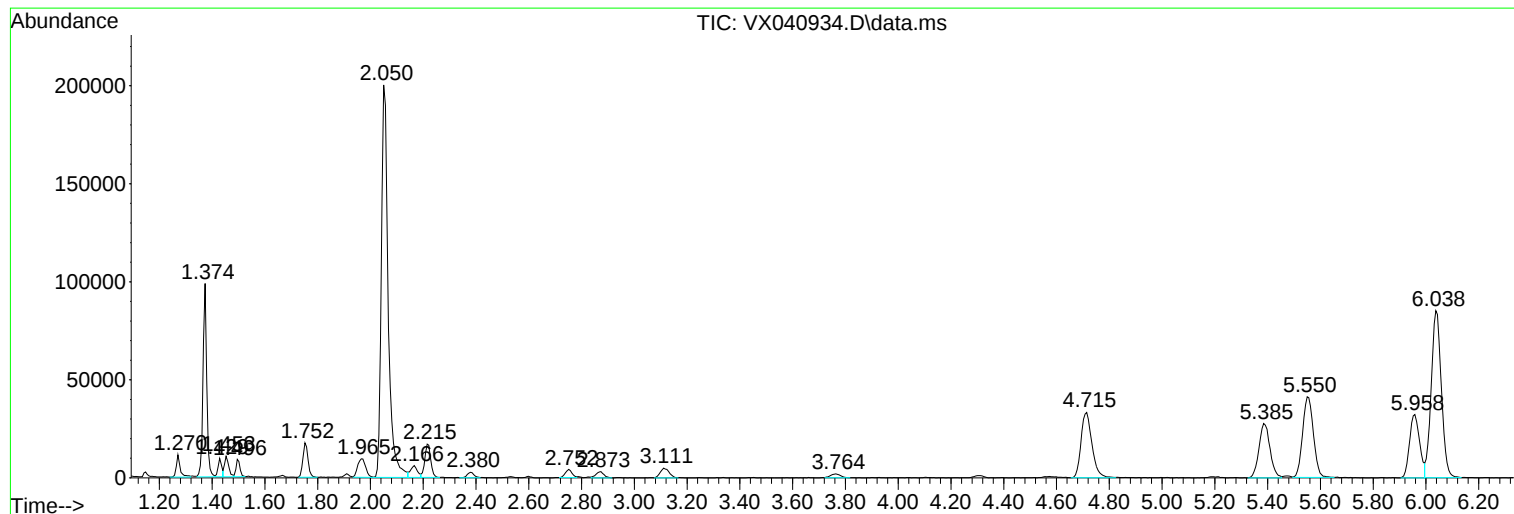
Sum of corrected areas: 3325279

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040824\
Data File : VX040934.D
Acq On : 08 Apr 2024 16:54
Operator : JC/MD
Sample : P2026-04 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50313

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040824\
Data File : VX040934.D
Acq On : 08 Apr 2024 16:54
Operator : JC/MD
Sample : P2026-04 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50313

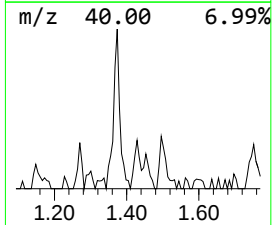
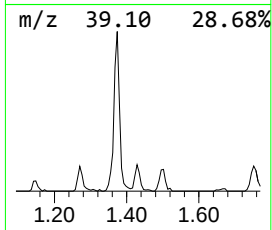
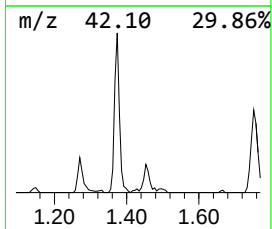
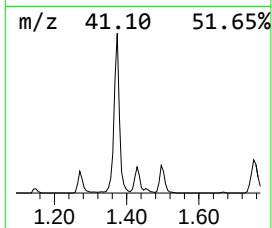
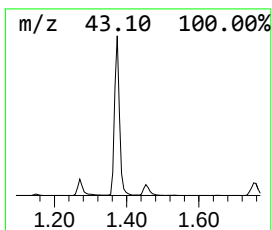
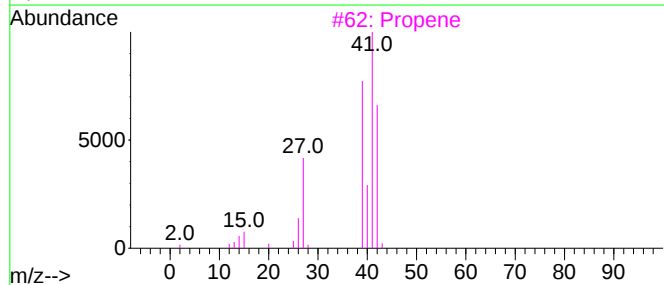
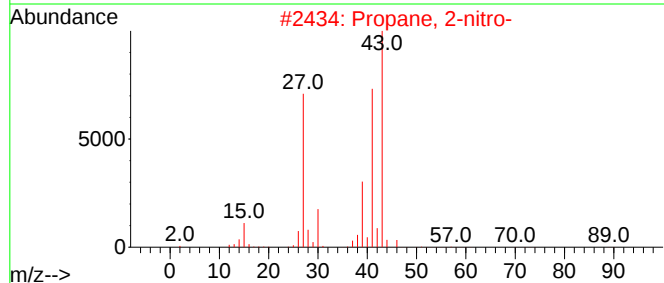
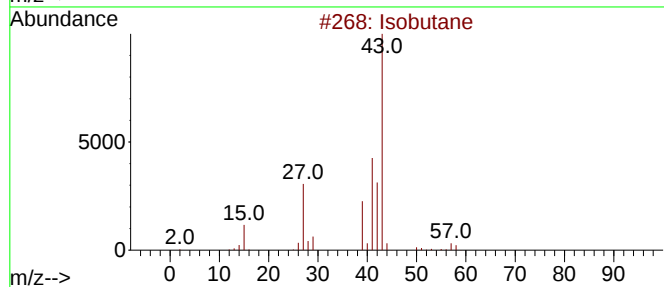
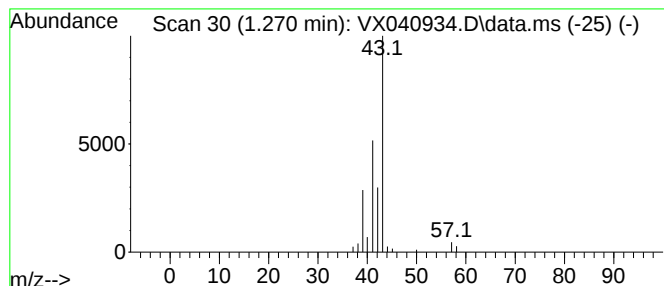
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040124W.M
Quant Title : SW846 8260

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

Peak Number 1 Isobutane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.270	5.12 ug/l	11939	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutane	58	C4H10	000075-28-5	56
2			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	9
3			Propene	42	C3H6	000115-07-1	7
4			Hydrogen isocyanate	43	CHNO	000075-13-8	4
5			1-Butanol	74	C4H10O	000071-36-3	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040824\
Data File : VX040934.D
Acq On : 08 Apr 2024 16:54
Operator : JC/MD
Sample : P2026-04 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50313

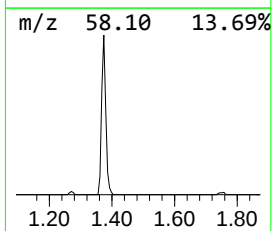
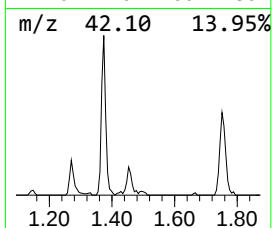
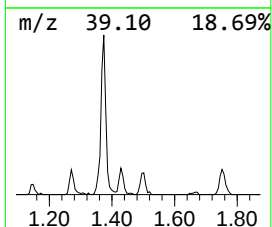
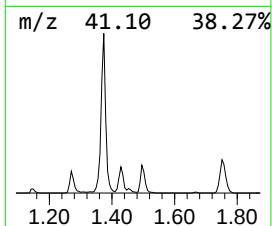
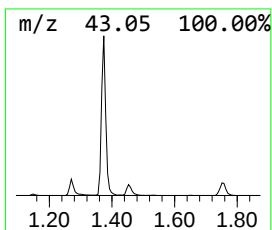
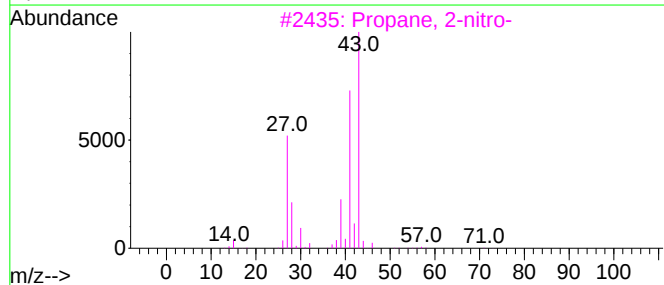
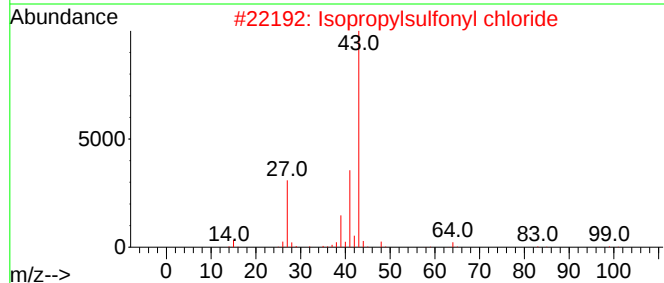
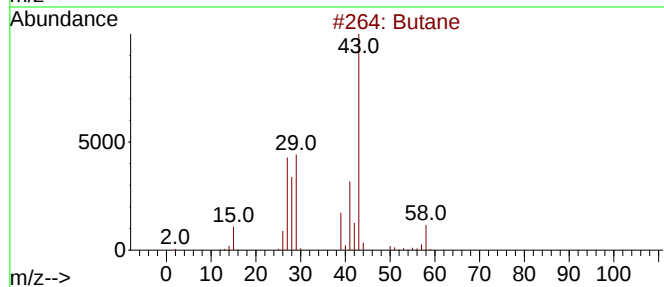
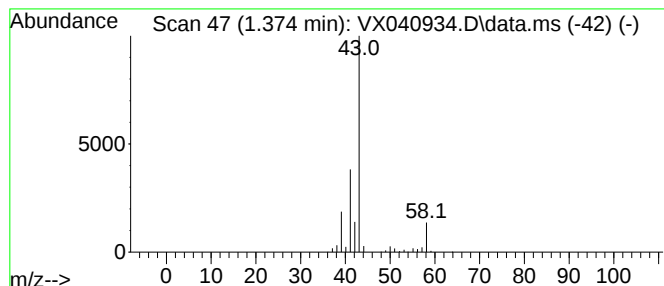
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040124W.M
Quant Title : SW846 8260

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	41.58 ug/l	96983	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			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5			Diazene, dimethyl-	58	C2H6N2	000503-28-6	5



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040824\
Data File : VX040934.D
Acq On : 08 Apr 2024 16:54
Operator : JC/MD
Sample : P2026-04 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50313

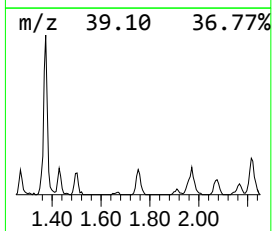
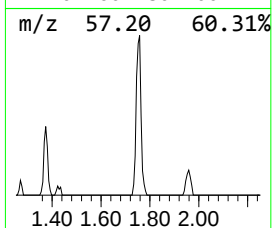
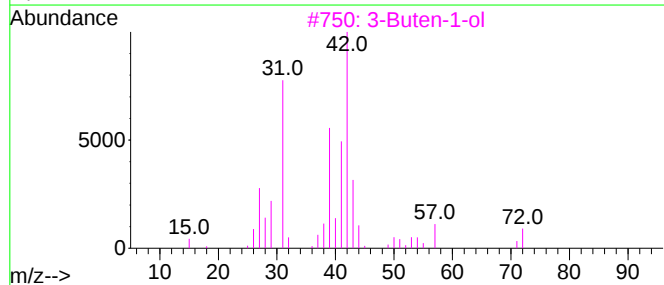
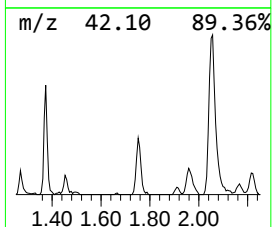
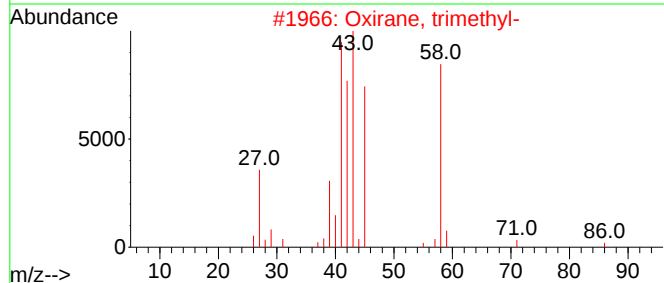
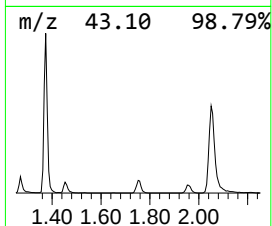
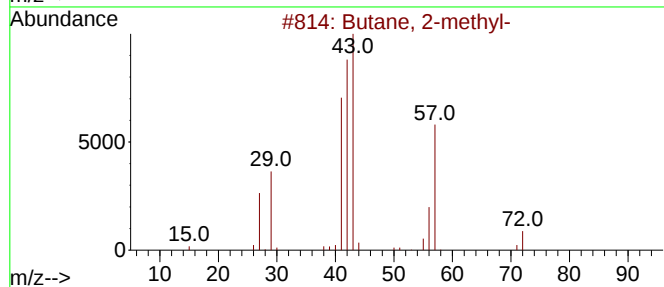
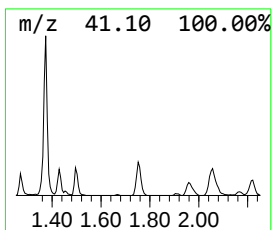
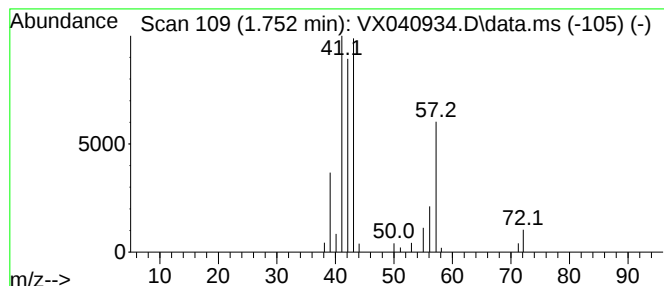
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040124W.M
Quant Title : SW846 8260

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

Peak Number 3 Butane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	10.10 ug/l	23551	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	90
2			Oxirane, trimethyl-	86	C5H10O	005076-19-7	38
3			3-Buten-1-ol	72	C4H8O	000627-27-0	28
4			Pentane, 2-bromo-	150	C5H11Br	000107-81-3	23
5			Pentane	72	C5H12	000109-66-0	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040824\
Data File : VX040934.D
Acq On : 08 Apr 2024 16:54
Operator : JC/MD
Sample : P2026-04 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50313

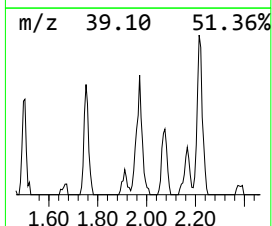
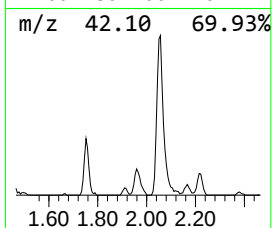
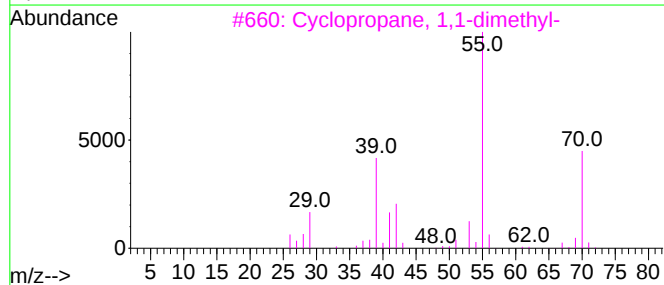
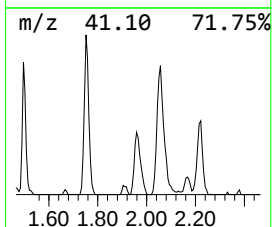
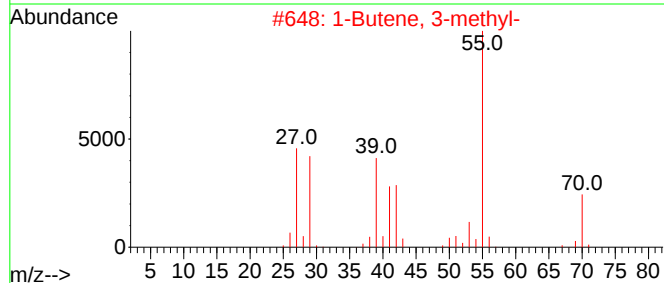
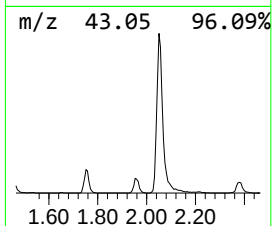
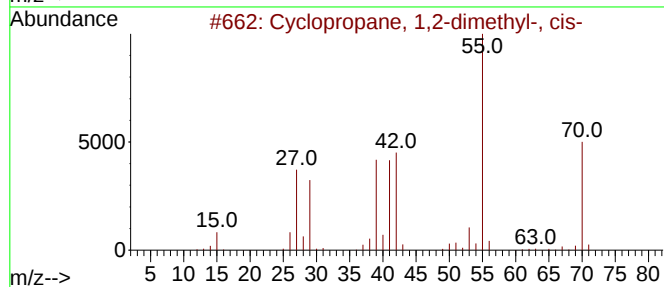
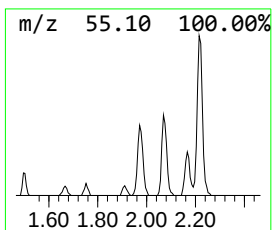
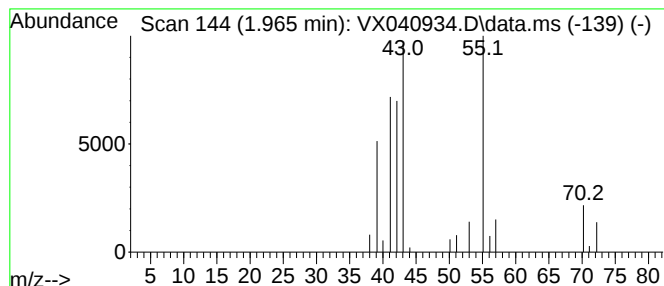
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040124W.M
Quant Title : SW846 8260

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

Peak Number 4 Cyclopropane, 1,2-dimethyl-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.965	8.47 ug/l	19746	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	53
2			1-Butene, 3-methyl-	70	C5H10	000563-45-1	52
3			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	50
4			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	45
5			2-Pentene, (E)-	70	C5H10	000646-04-8	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040824\
Data File : VX040934.D
Acq On : 08 Apr 2024 16:54
Operator : JC/MD
Sample : P2026-04 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50313

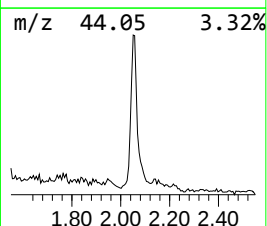
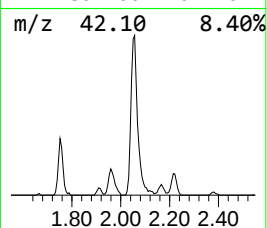
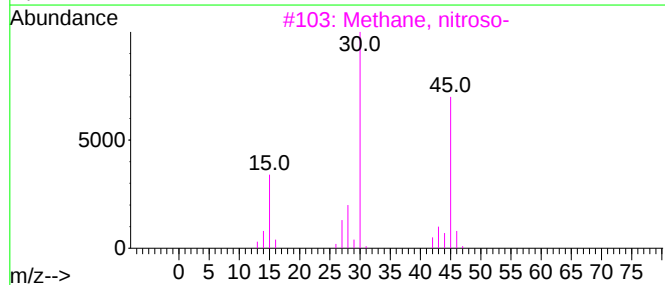
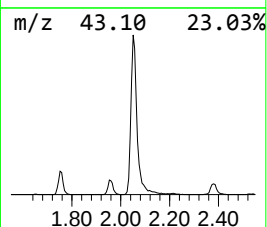
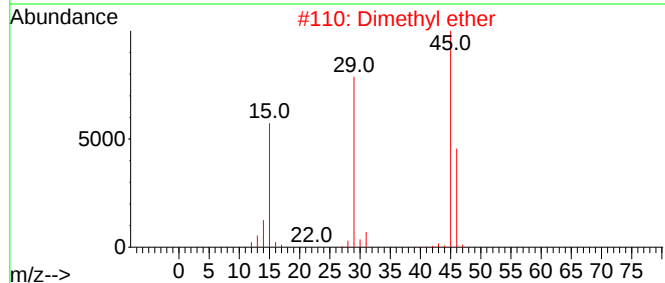
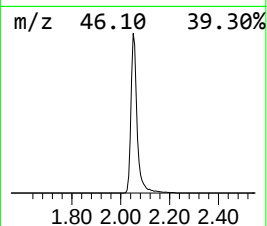
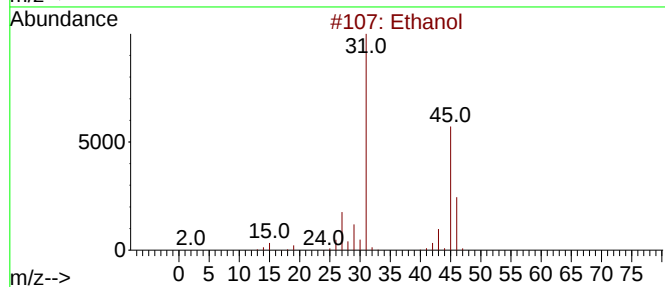
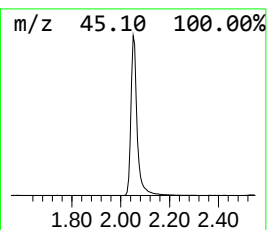
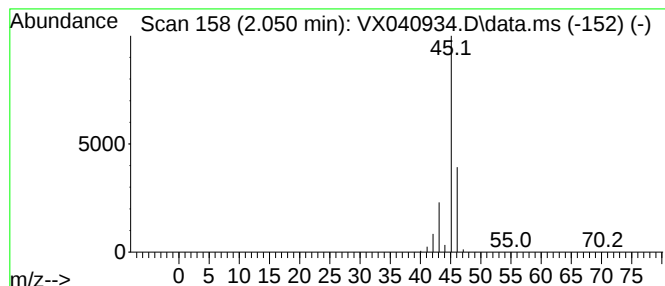
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040124W.M
Quant Title : SW846 8260

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

Peak Number 5 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.050	153.45 ug/l	357913	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			Oxalic acid	90	C2H2O4	000144-62-7	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040824\
Data File : VX040934.D
Acq On : 08 Apr 2024 16:54
Operator : JC/MD
Sample : P2026-04 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50313

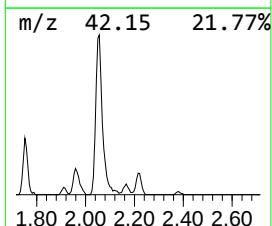
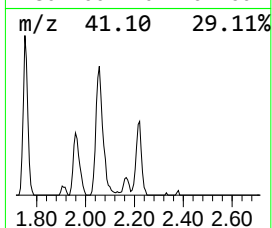
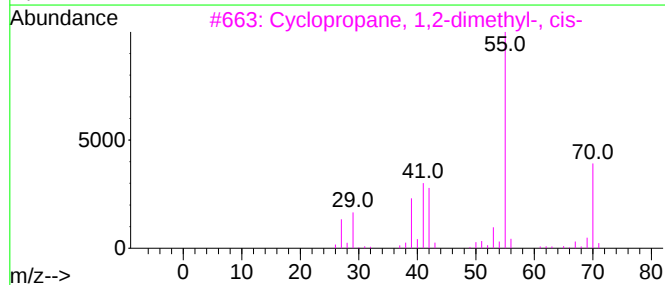
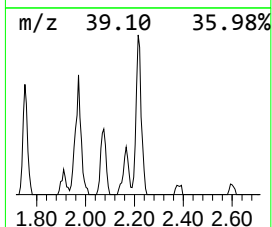
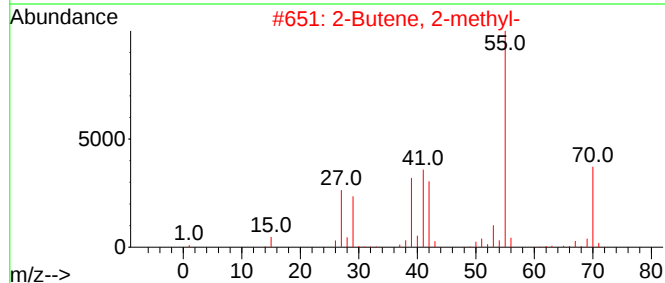
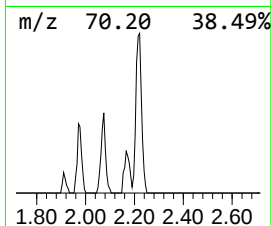
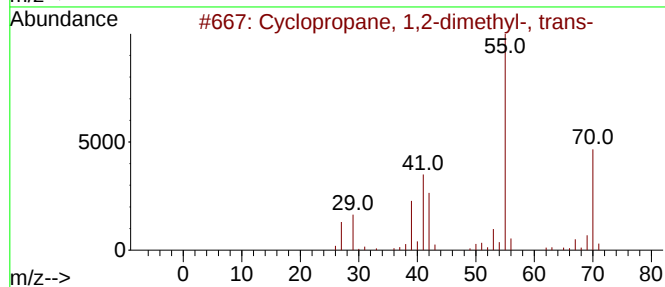
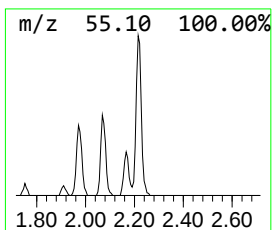
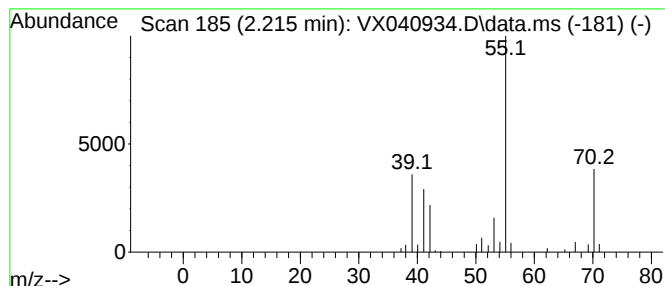
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040124W.M
Quant Title : SW846 8260

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

Peak Number 6 Cyclopropane, 1,2-dimethyl-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	11.31 ug/l	26386	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	90
2			2-Butene, 2-methyl-	70	C5H10	000513-35-9	90
3			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	86
4			1-Butene, 3-methyl-	70	C5H10	000563-45-1	86
5			2-Methyl-1-butene	70	C5H10	000563-46-2	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040824\
Data File : VX040934.D
Acq On : 08 Apr 2024 16:54
Operator : JC/MD
Sample : P2026-04 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50313

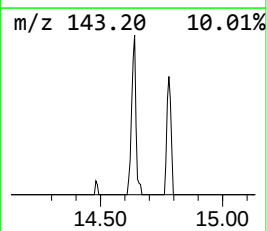
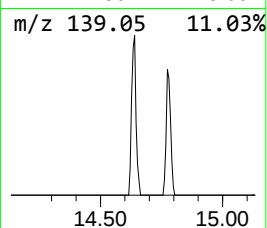
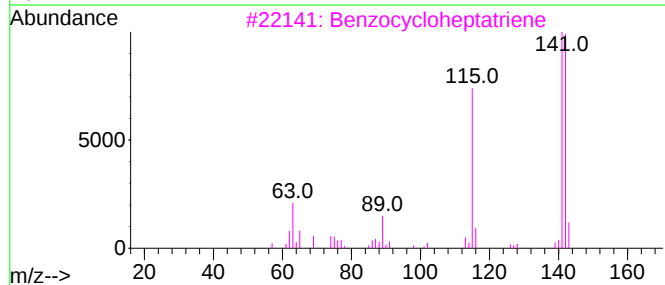
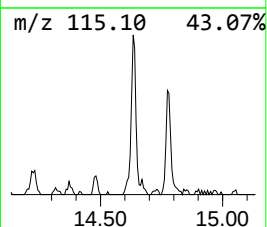
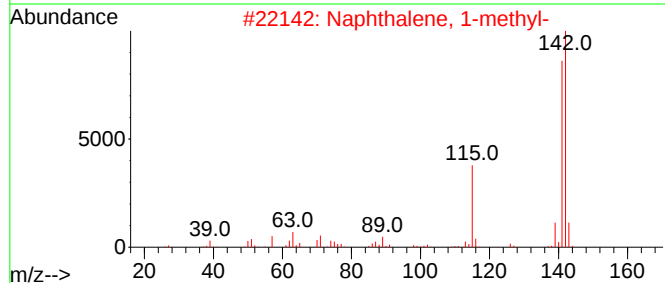
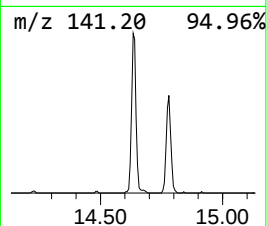
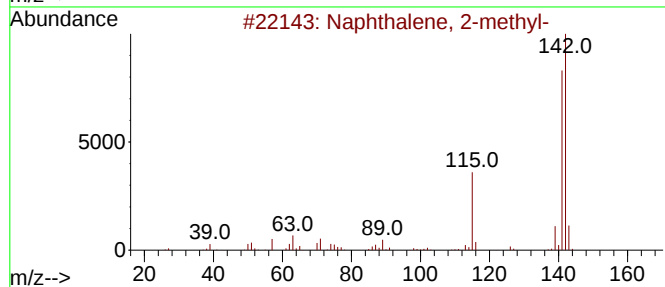
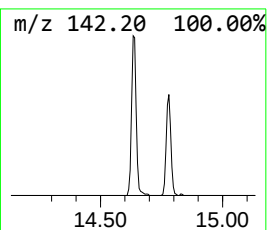
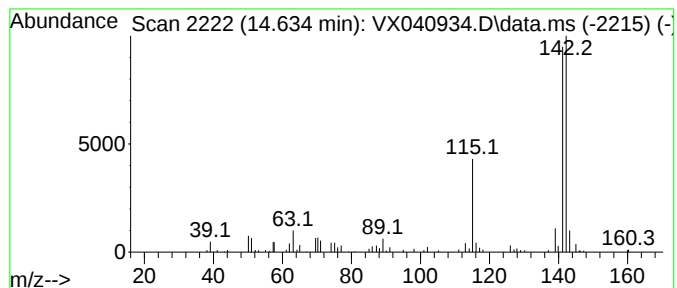
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040124W.M
Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.634	10.21 ug/l	51259	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
3			Benzocycloheptatriene	142	C11H10	000264-09-5	94
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\WX040824\
Data File : VX040934.D
Acq On : 08 Apr 2024 16:54
Operator : JC/MD
Sample : P2026-04 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50313

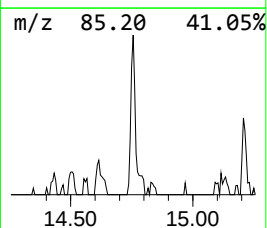
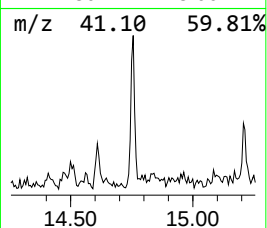
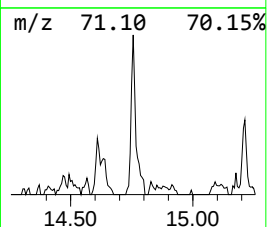
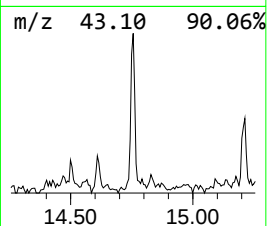
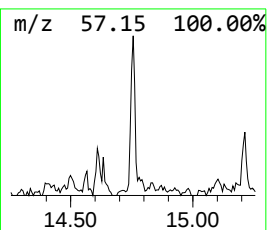
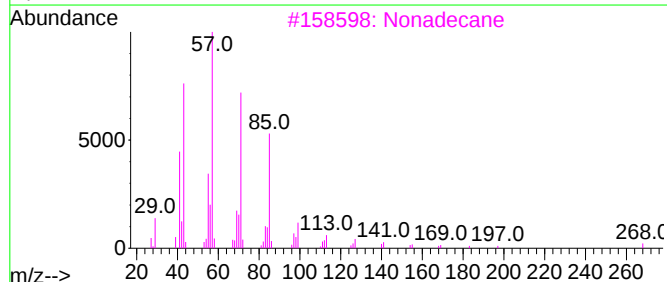
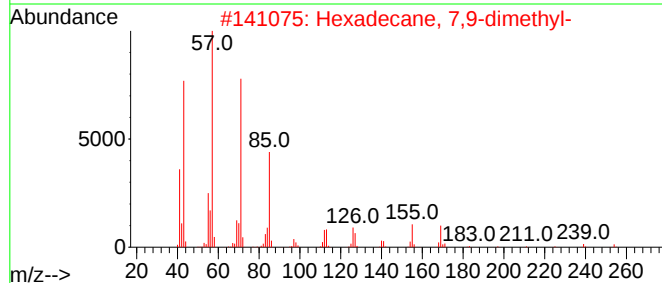
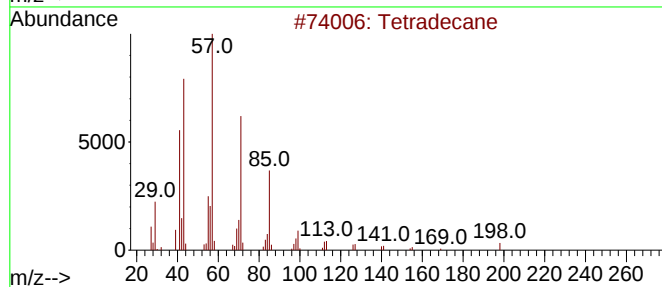
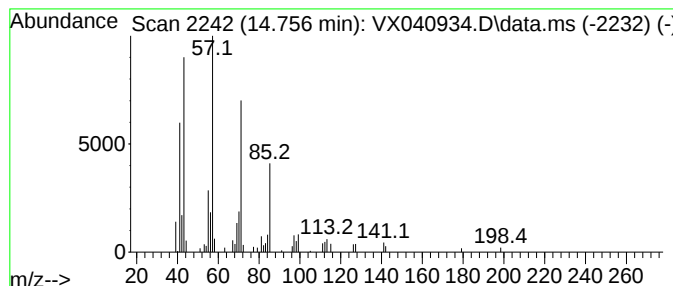
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040124W.M
Quant Title : SW846 8260

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

Peak Number 8 Tetradecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.756	5.17 ug/l	25927	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane	198	C14H30	000629-59-4	87
2		Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	86
3		Nonadecane	268	C19H40	000629-92-5	83
4		Tridecane	184	C13H28	000629-50-5	80
5		Hexadecane	226	C16H34	000544-76-3	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040824\
Data File : VX040934.D
Acq On : 08 Apr 2024 16:54
Operator : JC/MD
Sample : P2026-04 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50313

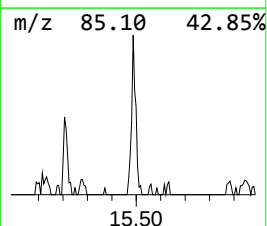
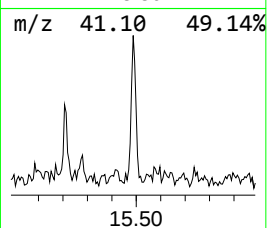
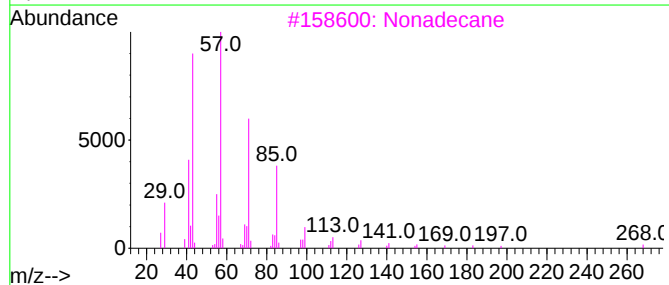
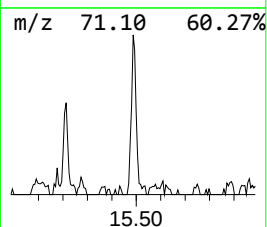
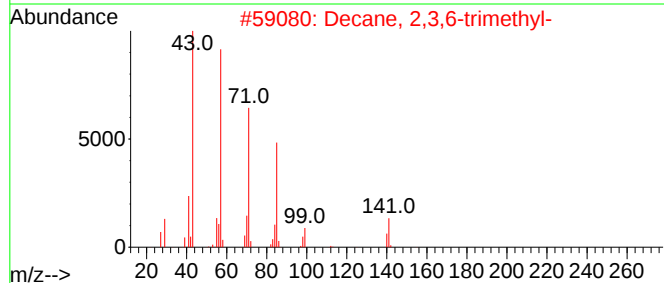
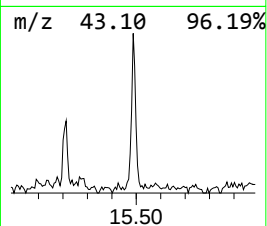
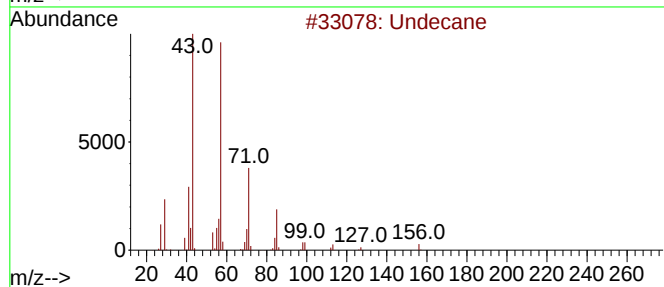
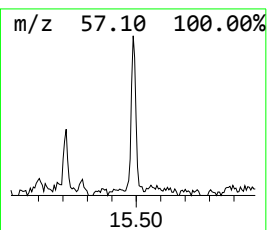
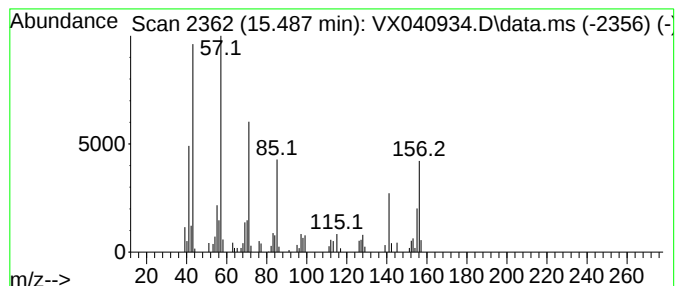
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040124W.M
Quant Title : SW846 8260

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

Peak Number 9 Undecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.487	6.45 ug/l	32372	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	58
2	Decane, 2,3,6-trimethyl-			184	C13H28	062238-12-4	46
3	Nonadecane			268	C19H40	000629-92-5	45
4	Hexadecane			226	C16H34	000544-76-3	43
5	Pentadecane			212	C15H32	000629-62-9	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040824\
Data File : VX040934.D
Acq On : 08 Apr 2024 16:54
Operator : JC/MD
Sample : P2026-04 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50313

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
Isobutane	1.270	5.1	ug/l	11939	1	5.550	116624	50.0
Butane	1.374	41.6	ug/l	96983	1	5.550	116624	50.0
Butane, 2-methyl-	1.752	10.1	ug/l	23551	1	5.550	116624	50.0
Cyclopropane, 1...	1.965	8.5	ug/l	19746	1	5.550	116624	50.0
Ethanol	2.050	153.4	ug/l	357913	1	5.550	116624	50.0
Cyclopropane, 1...	2.215	11.3	ug/l	26386	1	5.550	116624	50.0
Naphthalene, 2-...	14.634	10.2	ug/l	51259	4	12.024	250947	50.0
Tetradecane	14.756	5.2	ug/l	25927	4	12.024	250947	50.0
Undecane	15.487	6.5	ug/l	32372	4	12.024	250947	50.0