

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120622\
 Data File : VX033269.D
 Acq On : 06 Dec 2022 19:18
 Operator : JC/MD
 Sample : N5859-04
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 ORA-0583

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\82X112222W.M
 Title : SW846 8260

Signal : TIC: VX033269.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	23	rVB	190392	188596	32.75%	3.010%
2	1.264	25	29	38	rBV	35938	36413	6.32%	0.581%
3	1.368	41	46	53	rBV	43958	53322	9.26%	0.851%
4	1.752	104	109	115	rVB	11651	15790	2.74%	0.252%
5	1.953	138	142	154	rVB	5524	8387	1.46%	0.134%
6	2.136	159	172	175	rBV3	8376	22358	3.88%	0.357%
7	2.392	207	214	228	rVB	22245	47264	8.21%	0.754%
8	2.593	236	247	262	rBV2	6392	30675	5.33%	0.490%
9	2.709	262	266	274	rVB	3657	6881	1.19%	0.110%
10	2.965	299	308	325	rBV6	12001	40243	6.99%	0.642%
11	3.331	359	368	375	rBV2	4277	9638	1.67%	0.154%
12	3.697	412	428	442	rBV	72892	201771	35.04%	3.220%
13	3.928	454	466	467	rBV3	4135	10653	1.85%	0.170%
14	4.227	503	515	531	rBV	145957	400859	69.61%	6.398%
15	4.562	561	570	585	rBV	46282	135058	23.45%	2.156%
16	5.385	694	705	717	rBV2	70863	205965	35.77%	3.287%
17	5.556	722	733	745	rVB	142079	401473	69.71%	6.407%
18	5.958	789	799	805	rBV2	67216	176010	30.56%	2.809%
19	6.038	805	812	824	rVB	112701	301203	52.30%	4.807%
20	6.763	922	931	950	rBB	210482	498476	86.56%	7.956%
21	7.251	1003	1011	1026	rBV2	10179	37480	6.51%	0.598%
22	7.580	1060	1065	1073	rVB2	11235	21310	3.70%	0.340%
23	8.647	1234	1240	1247	rBV	277052	440025	76.41%	7.023%
24	8.720	1247	1252	1258	rVV	176865	265576	46.12%	4.239%
25	8.775	1258	1261	1271	rVV2	7123	14969	2.60%	0.239%
26	9.250	1331	1339	1347	rBV3	5931	13938	2.42%	0.222%
27	9.488	1373	1378	1384	rBV2	9304	14230	2.47%	0.227%
28	10.055	1465	1471	1483	rBV	439950	575883	100.00%	9.191%
29	10.159	1483	1488	1491	rBV2	5117	7839	1.36%	0.125%
30	10.195	1491	1494	1499	rVB	12533	17171	2.98%	0.274%
31	10.299	1506	1511	1517	rVB	67739	93528	16.24%	1.493%
32	10.445	1528	1535	1540	rVB	44265	57802	10.04%	0.923%
33	10.506	1541	1545	1553	rVB2	6424	8955	1.56%	0.143%
34	10.640	1561	1567	1572	rBV	27797	41917	7.28%	0.669%
35	10.756	1581	1586	1596	rBV4	9811	18691	3.25%	0.298%
36	11.079	1634	1639	1645	rBV	282039	369058	64.09%	5.890%

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Integration Parameters: RTEINT.P

Integrator: RTE

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37	11.378	1682	1688	1694	rBV2	10111	19729	3.43%	0.315%
38	11.451	1698	1700	1707	rVB	8315	10594	1.84%	0.169%
39	11.573	1713	1720	1723	rBV2	6369	9054	1.57%	0.145%
40	11.616	1723	1727	1729	rBV3	6694	10104	1.75%	0.161%
41	11.683	1734	1738	1745	rVB	14284	17808	3.09%	0.284%
42	11.750	1745	1749	1755	rBV	22729	31702	5.50%	0.506%
43	11.988	1780	1788	1789	rBV5	5229	8626	1.50%	0.138%
44	12.024	1789	1794	1801	rVV	439960	560318	97.30%	8.943%
45	12.085	1801	1804	1809	rVB	8583	11036	1.92%	0.176%
46	12.219	1821	1826	1837	rBV	302173	444560	77.20%	7.095%
47	12.311	1837	1841	1852	rVV4	20458	45931	7.98%	0.733%
48	12.415	1854	1858	1863	rVB2	14669	19806	3.44%	0.316%
49	12.567	1879	1883	1886	rBV5	5752	8447	1.47%	0.135%
50	12.762	1912	1915	1918	rBV3	5070	8262	1.43%	0.132%
51	12.799	1918	1921	1926	rVV6	6717	11577	2.01%	0.185%
52	12.847	1926	1929	1933	rVB	5222	5764	1.00%	0.092%
53	12.963	1945	1948	1955	rVB6	3814	6398	1.11%	0.102%
54	13.286	1992	2001	2007	rVB4	5452	10632	1.85%	0.170%
55	13.420	2017	2023	2028	rBV4	4402	7336	1.27%	0.117%
56	13.750	2073	2077	2078	rBV	16260	16238	2.82%	0.259%
57	13.774	2078	2081	2086	rVV	40697	58993	10.24%	0.942%
58	13.847	2089	2093	2100	rVV	20413	32531	5.65%	0.519%
59	13.914	2100	2104	2113	rVB2	22715	34037	5.91%	0.543%
60	14.134	2134	2140	2145	rBV	7466	11104	1.93%	0.177%
61	14.640	2218	2223	2229	rVB	20914	27917	4.85%	0.446%
62	14.780	2242	2246	2251	rVB	13034	15662	2.72%	0.250%
63	15.969	2436	2441	2451	rBV3	17604	32137	5.58%	0.513%

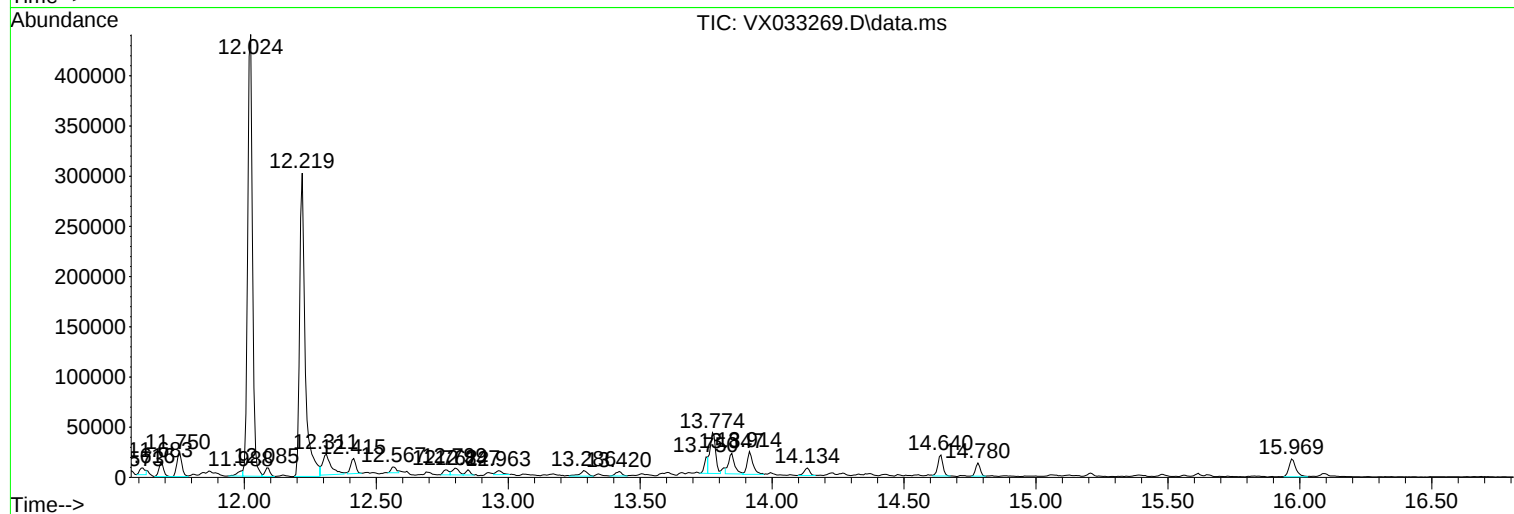
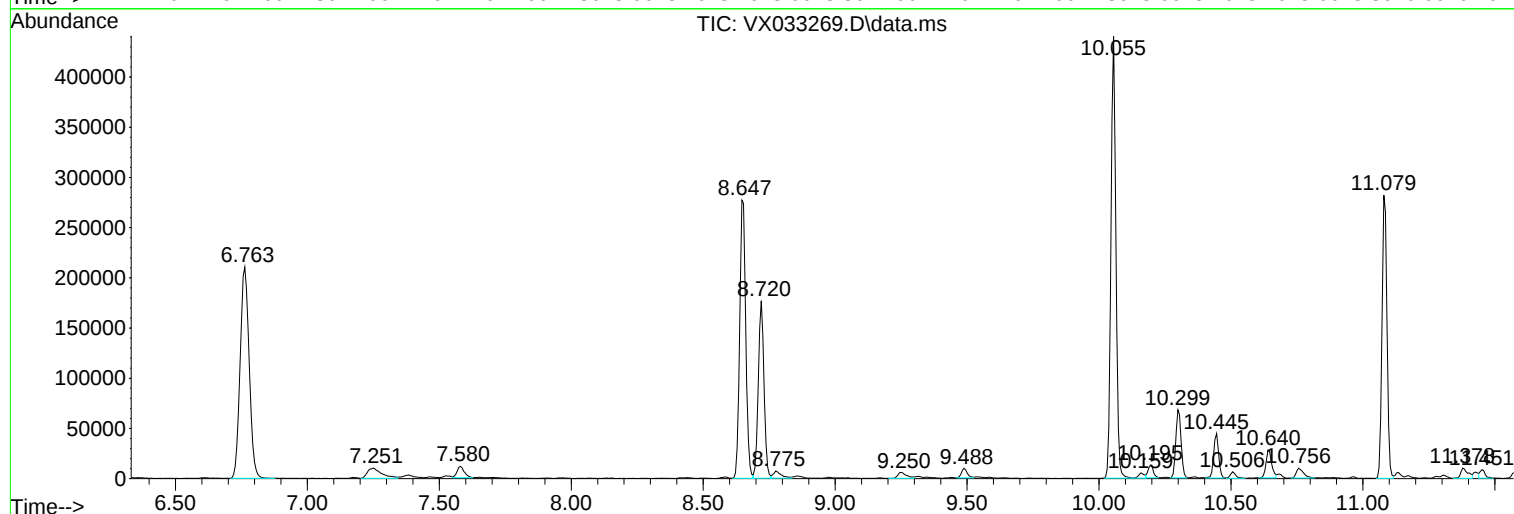
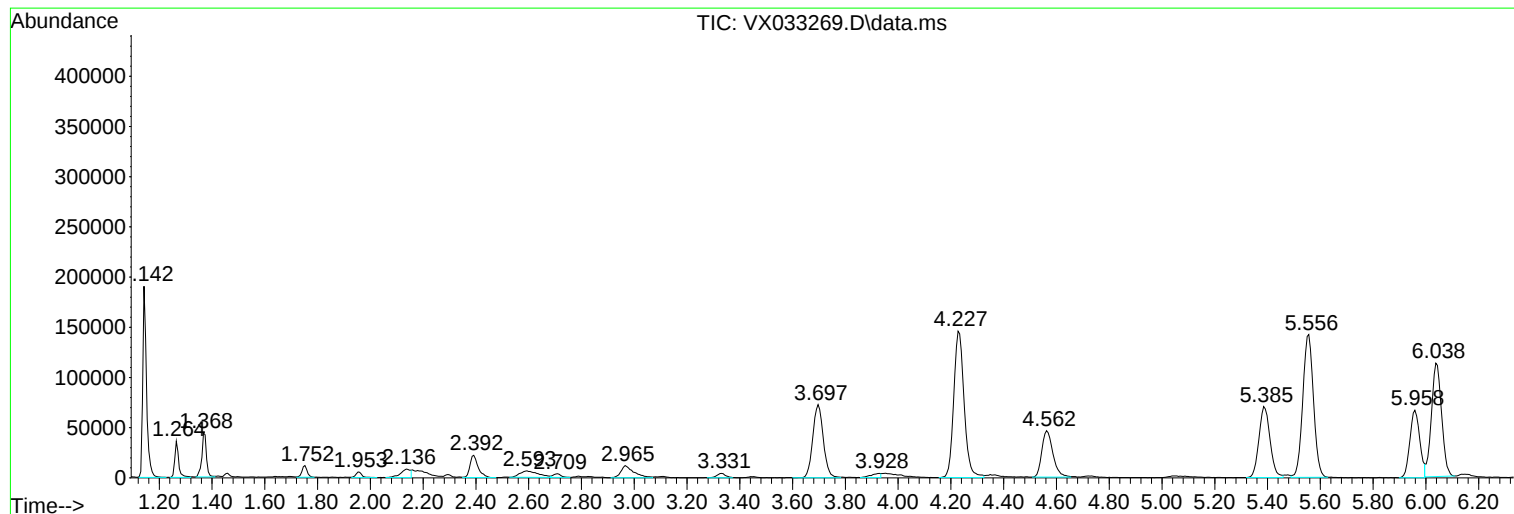
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Instrument :
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ClientSampleId :
ORA-0583

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_X
ClientSampleId :
ORA-0583

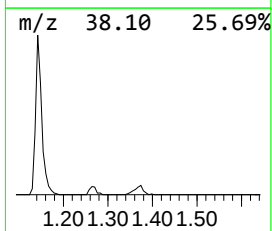
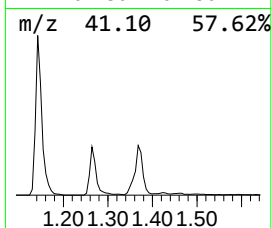
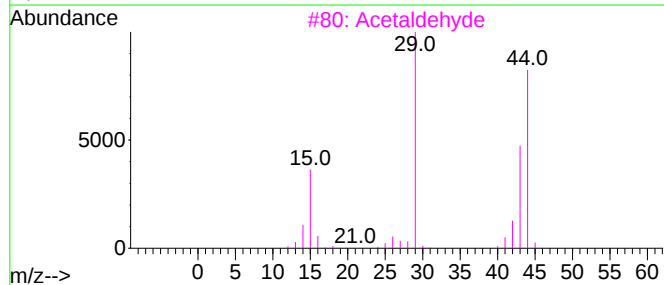
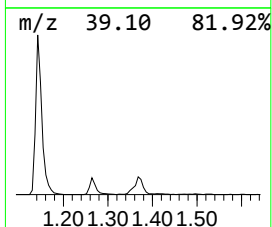
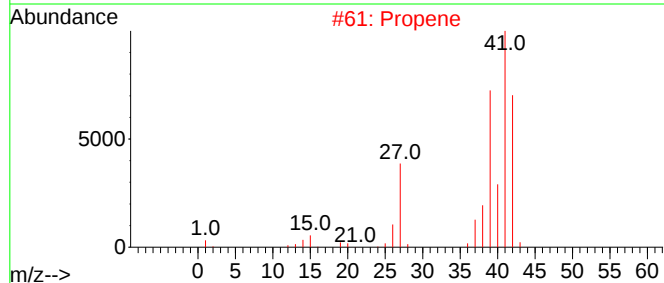
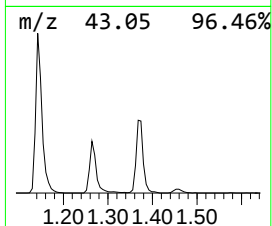
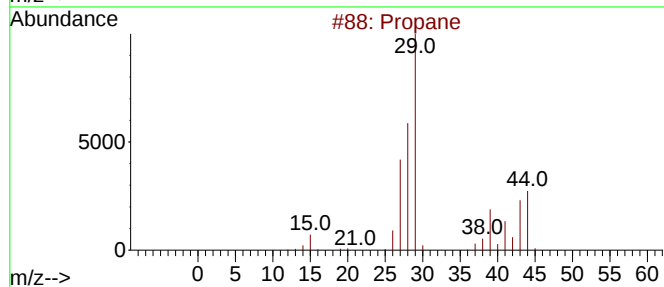
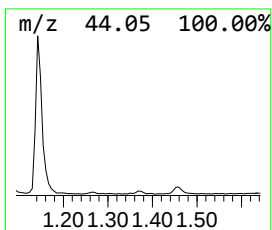
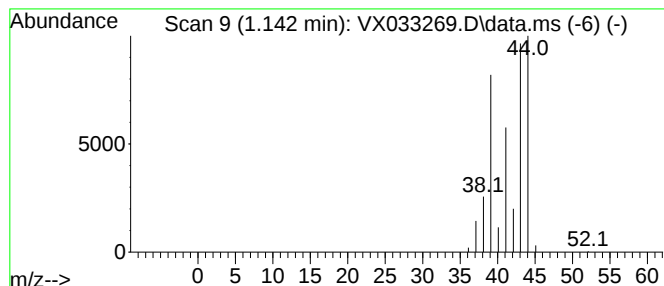
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

Peak Number 1 Propane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.142	23.49 ug/l	188596	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane			44	C3H8	000074-98-6	90
2	Propene			42	C3H6	000115-07-1	9
3	Acetaldehyde			44	C2H4O	000075-07-0	5
4	Cyclopropene			40	C3H4	002781-85-3	2
5	Alanine			89	C3H7NO2	000056-41-7	2



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ClientSampleId :
ORA-0583

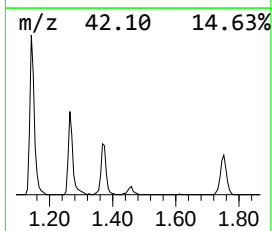
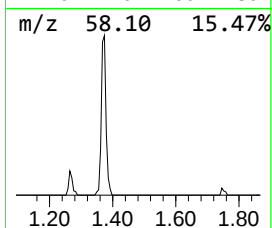
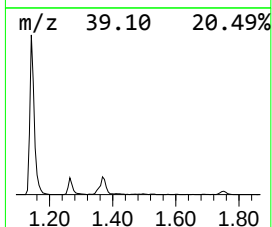
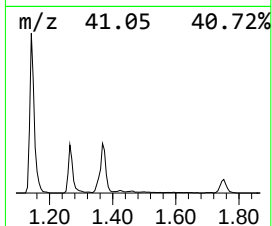
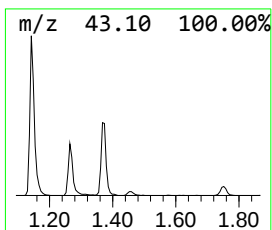
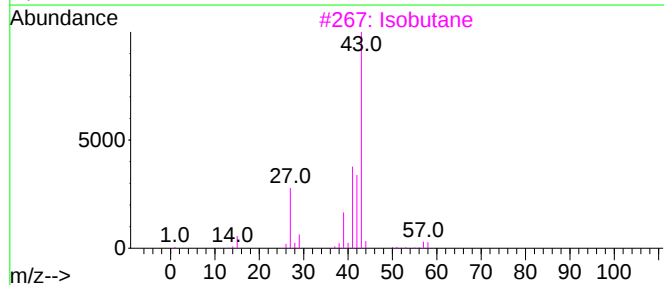
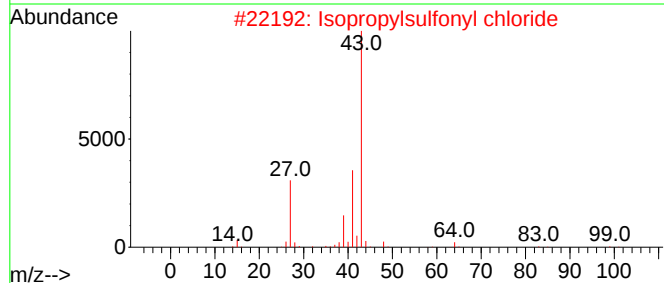
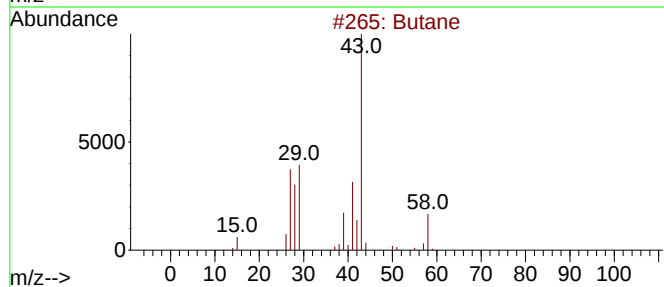
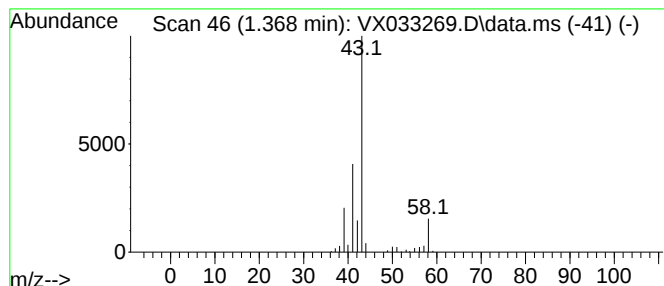
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.368	6.64 ug/l	53322	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	80
2			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
3			Isobutane	58	C4H10	000075-28-5	9
4			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5			Diazene, dimethyl-	58	C2H6N2	000503-28-6	5



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0583

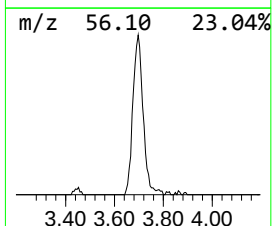
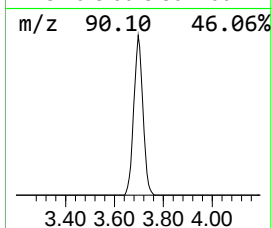
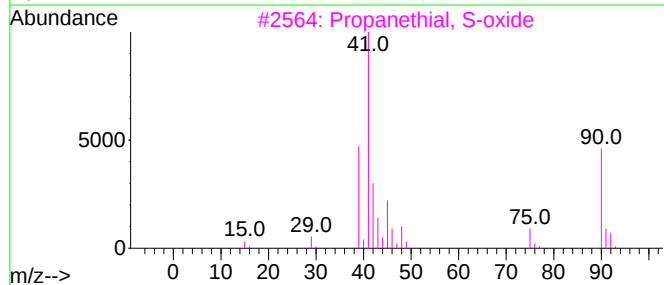
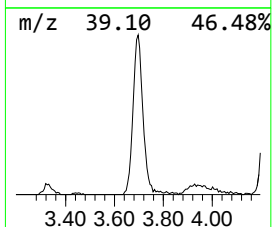
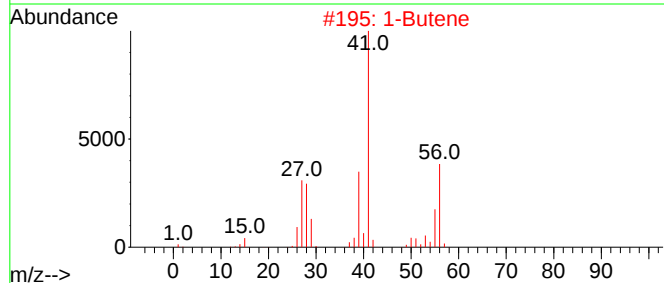
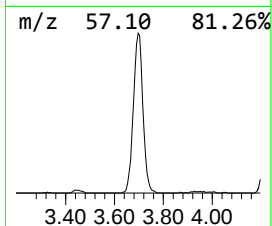
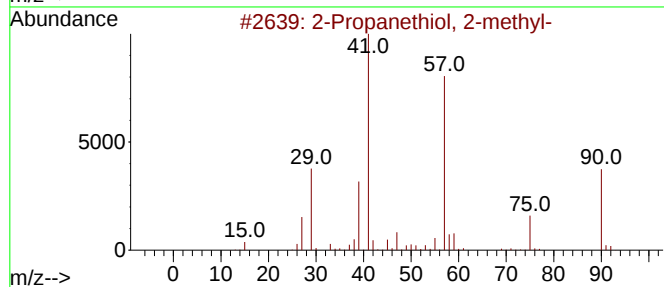
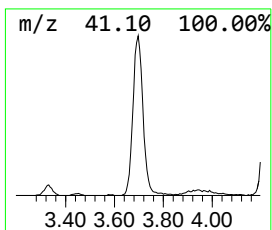
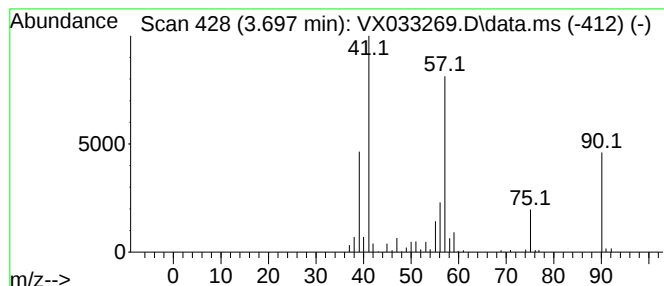
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.697	25.13 ug/l	201771	Pentafluorobenzene	5.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	50
2		1-Butene	56	C4H8	000106-98-9	38
3		Propanethial, S-oxide	90	C3H6OS	032157-29-2	38
4		1-Propene, 2-methyl-	56	C4H8	000115-11-7	38
5		Propane, 2-methyl-1-nitro-	103	C4H9NO2	000625-74-1	25



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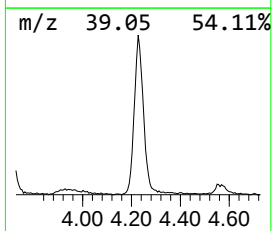
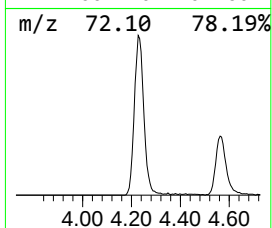
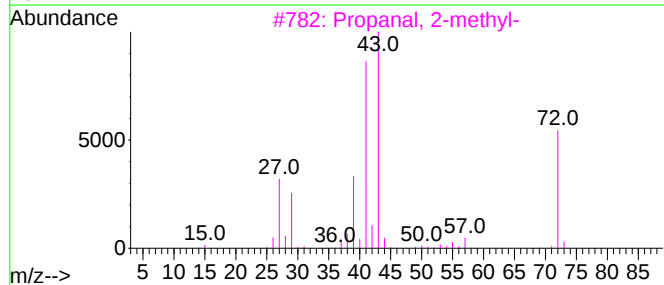
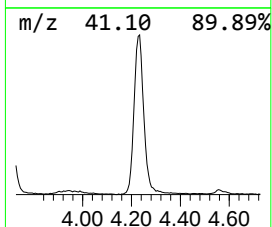
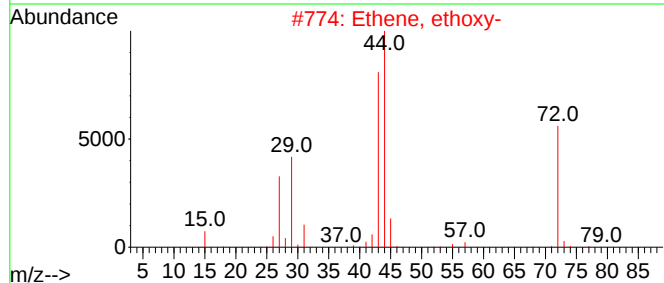
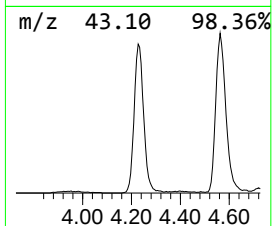
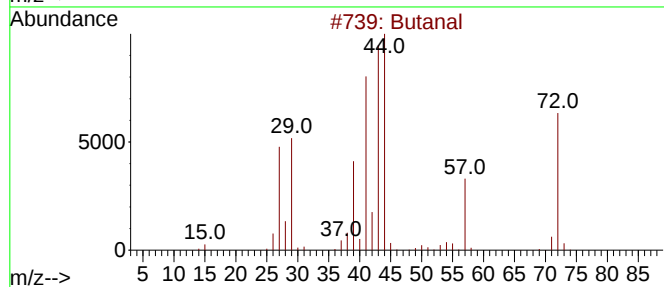
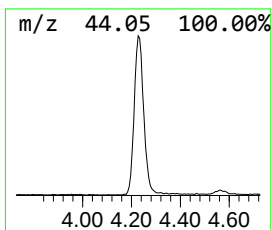
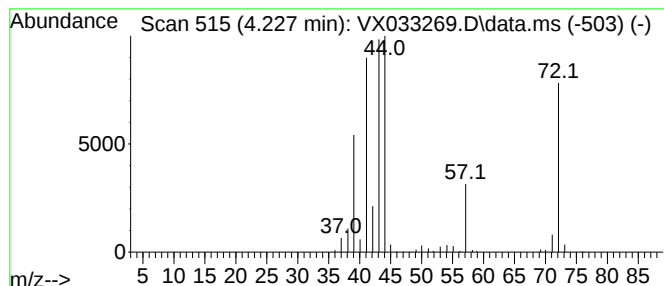
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

Peak Number 4 Butanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	49.92 ug/l	400859	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	52
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	46
4			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38
5			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37



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ClientSampleId :
ORA-0583

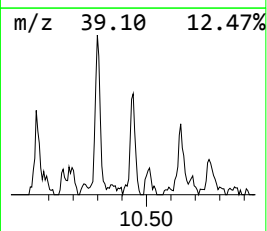
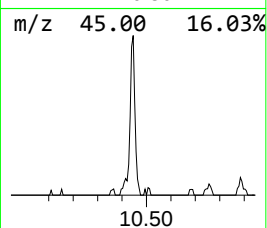
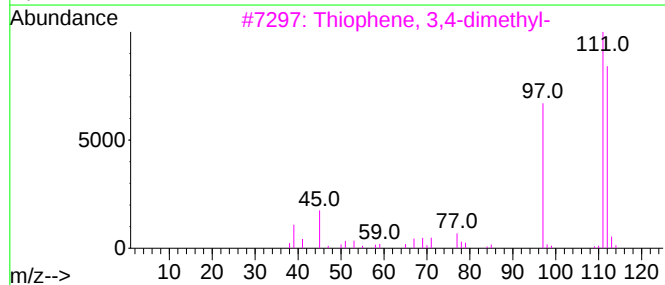
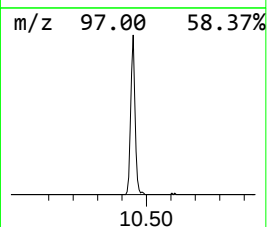
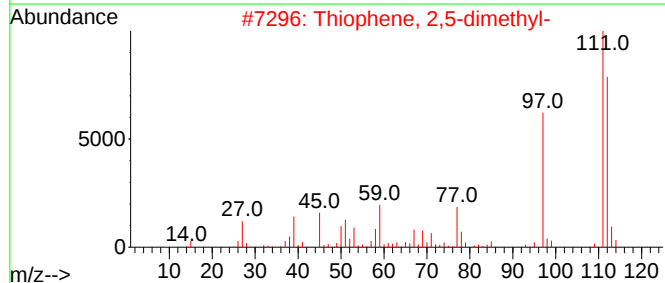
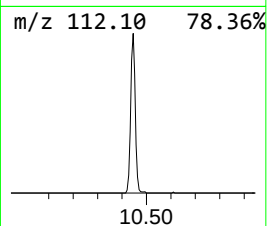
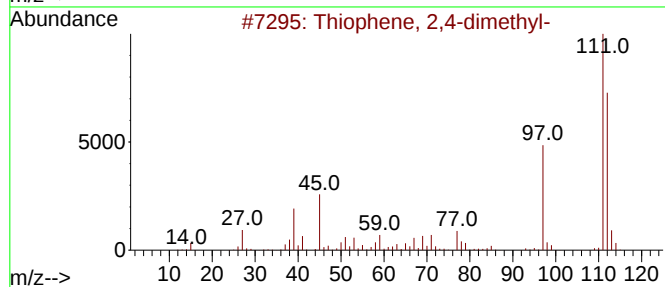
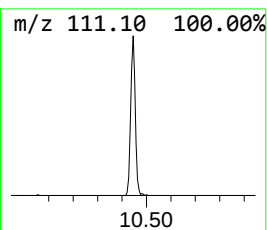
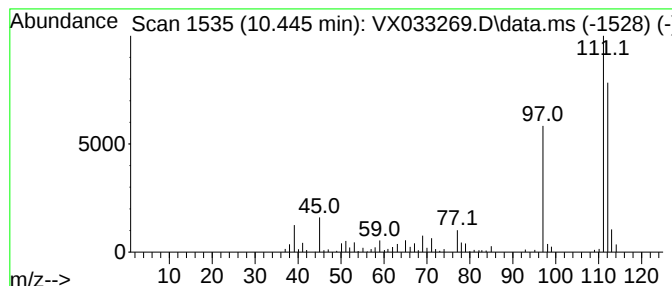
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Quant Title : SW846 8260

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

Peak Number 5 Thiophene, 2,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.445	5.02 ug/l	57802	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, 2,4-dimethyl-	112	C6H8S	000638-00-6	91
2			Thiophene, 2,5-dimethyl-	112	C6H8S	000638-02-8	90
3			Thiophene, 3,4-dimethyl-	112	C6H8S	000632-15-5	90
4			2-Thiophenecarboxaldehyde	112	C5H4OS	000098-03-3	59
5			Thiophene, 2,3-dimethyl-	112	C6H8S	000632-16-6	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120622\
Data File : VX033269.D
Acq On : 06 Dec 2022 19:18
Operator : JC/MD
Sample : N5859-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0583

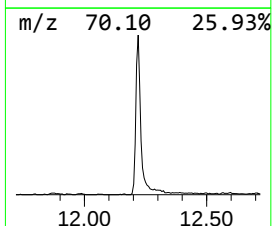
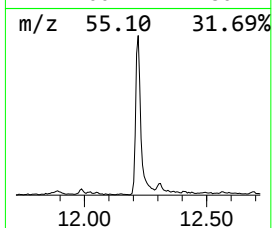
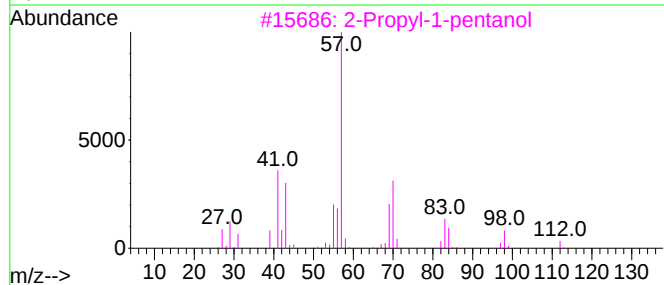
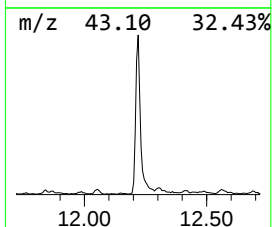
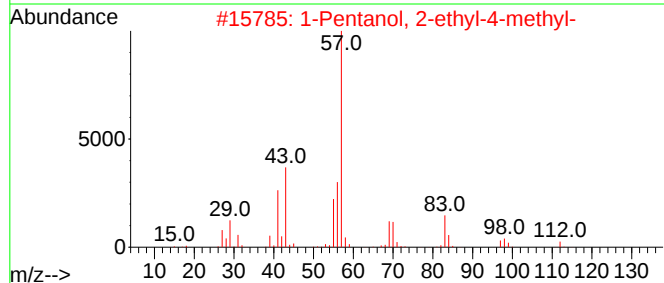
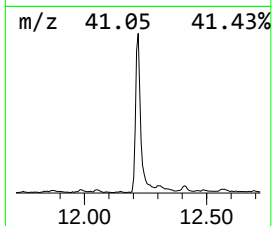
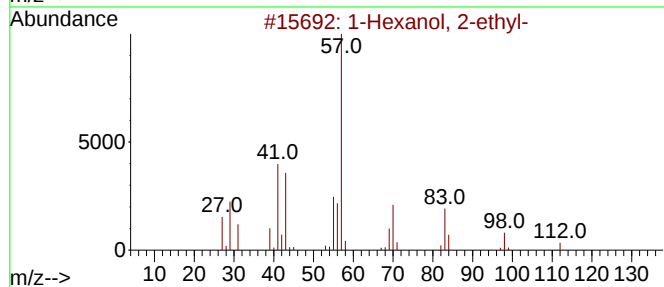
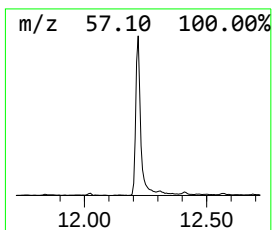
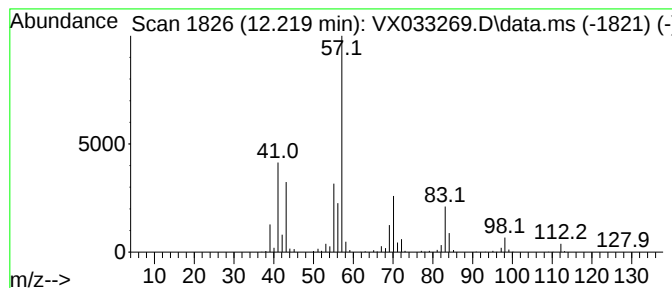
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	39.67 ug/l	444560	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	83
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5			Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120622\
Data File : VX033269.D
Acq On : 06 Dec 2022 19:18
Operator : JC/MD
Sample : N5859-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0583

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.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
Propane	1.142	23.5	ug/l	188596	1	5.556	401473	50.0
Butane	1.368	6.6	ug/l	53322	1	5.556	401473	50.0
2-Propanethiol,...	3.697	25.1	ug/l	201771	1	5.556	401473	50.0
Butanal	4.227	49.9	ug/l	400859	1	5.556	401473	50.0
Thiophene, 2,4-...	10.445	5.0	ug/l	57802	3	10.055	575883	50.0
1-Hexanol, 2-et...	12.219	39.7	ug/l	444560	4	12.024	560318	50.0