

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052421\
 Data File : VX022160.D
 Acq On : 24 May 2021 20:08
 Operator : JC/MD
 Sample : M2504-06
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-2

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\82X051921W.M
 Title : SW846 8260

Signal : TIC: VX022160.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	35	rBV	25555	39709	5.01%	0.864%
2	1.374	43	47	51	rVB	21692	21076	2.66%	0.458%
3	1.752	104	109	115	rBV	38728	52415	6.61%	1.140%
4	1.953	138	142	152	rVB	16978	27005	3.41%	0.587%
5	2.069	155	161	169	rBV3	5037	8127	1.02%	0.177%
6	2.337	197	205	211	rVV2	11733	22718	2.86%	0.494%
7	2.550	231	240	249	rVB3	4765	10567	1.33%	0.230%
8	2.782	270	278	284	rBV	35649	77342	9.75%	1.682%
9	2.959	300	307	318	rVB4	3653	11214	1.41%	0.244%
10	3.099	323	330	341	rBV3	5592	14683	1.85%	0.319%
11	4.306	522	528	538	rVB5	3661	10238	1.29%	0.223%
12	4.465	538	554	559	rBV5	3442	12750	1.61%	0.277%
13	5.397	695	707	718	rBV2	52854	152401	19.22%	3.314%
14	5.562	724	734	742	rBV2	80588	234335	29.55%	5.096%
15	5.970	790	801	814	rBV	63316	170021	21.44%	3.697%
16	6.257	836	848	874	rVB	259400	793065	100.00%	17.247%
17	6.769	922	932	943	rBV2	146043	347378	43.80%	7.554%
18	7.373	1025	1031	1038	rBV4	3671	9135	1.15%	0.199%
19	7.610	1059	1070	1077	rBV	10399	23758	3.00%	0.517%
20	7.775	1090	1097	1106	rVB4	5712	10941	1.38%	0.238%
21	7.988	1123	1132	1143	rVB	167653	331921	41.85%	7.218%
22	8.110	1143	1152	1163	rBV	134885	264716	33.38%	5.757%
23	8.433	1201	1205	1212	rVV2	7460	12049	1.52%	0.262%
24	8.653	1230	1241	1250	rBV	310081	494247	62.32%	10.748%
25	9.244	1332	1338	1348	rBV	58711	96079	12.11%	2.089%
26	9.458	1366	1373	1379	rBV5	8982	17358	2.19%	0.377%
27	9.945	1448	1453	1460	rBV2	7624	12086	1.52%	0.263%
28	10.055	1466	1471	1478	rVB	281389	395990	49.93%	8.612%
29	10.201	1490	1495	1499	rBV	12059	15727	1.98%	0.342%
30	10.305	1506	1512	1519	rVB	29596	39856	5.03%	0.867%
31	11.085	1634	1640	1650	rVV	230118	289840	36.55%	6.303%
32	11.384	1685	1689	1691	rBV	8568	12015	1.52%	0.261%
33	11.457	1697	1701	1706	rBV2	6716	8336	1.05%	0.181%
34	11.713	1737	1743	1746	rBV3	6203	8432	1.06%	0.183%
35	11.756	1746	1750	1755	rVB	24303	28472	3.59%	0.619%
36	12.024	1789	1794	1800	rVB	293241	351667	44.34%	7.648%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052421\
Data File : VX022160.D
Acq On : 24 May 2021 20:08
Operator : JC/MD
Sample : M2504-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

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\82X051921W.M
Title : SW846 8260

37	12.250	1825	1831	1838	rBV	26177	34690	4.37%	0.754%
38	12.317	1838	1842	1849	rVB2	6319	9004	1.14%	0.196%
39	12.707	1901	1906	1912	rBV4	7572	12461	1.57%	0.271%
40	13.030	1955	1959	1965	rVB3	6086	9474	1.19%	0.206%
41	13.122	1969	1974	1976	rBV2	12944	18969	2.39%	0.413%
42	13.237	1990	1993	1998	rVB3	11056	12976	1.64%	0.282%
43	13.298	1998	2003	2007	rVB3	9045	12873	1.62%	0.280%
44	13.542	2040	2043	2048	rVB	12298	14514	1.83%	0.316%
45	13.646	2053	2060	2061	rVV3	8773	15522	1.96%	0.338%
46	13.664	2061	2063	2069	rVB	15738	18781	2.37%	0.408%
47	13.780	2074	2082	2089	rBV	5958	11391	1.44%	0.248%

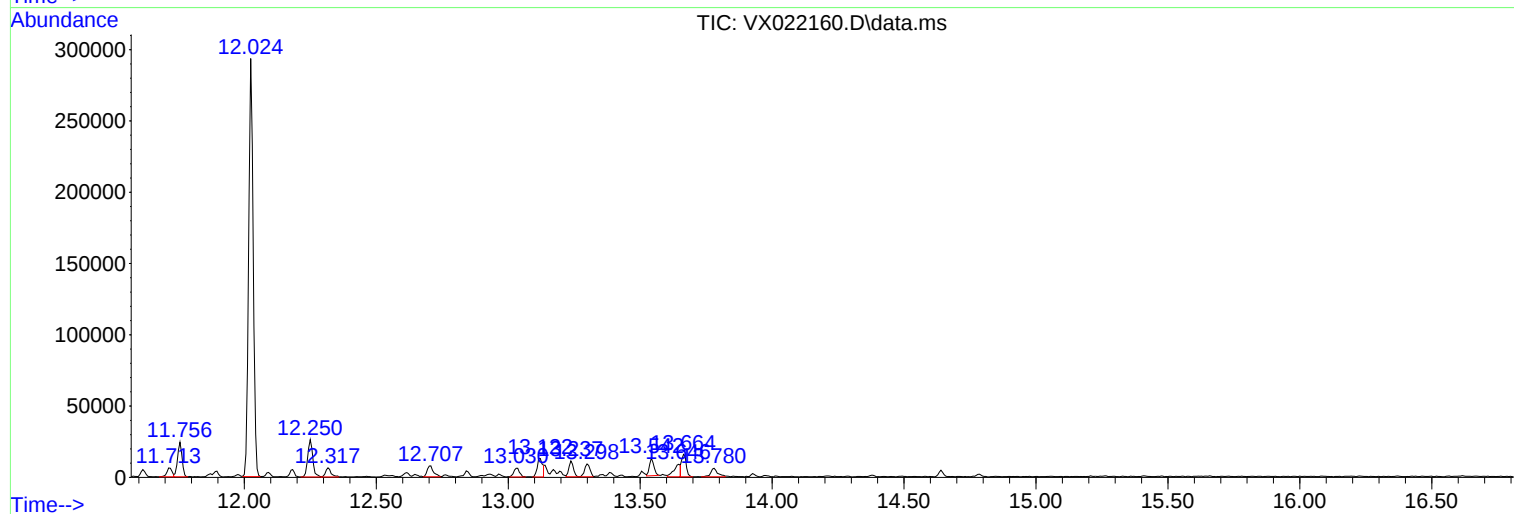
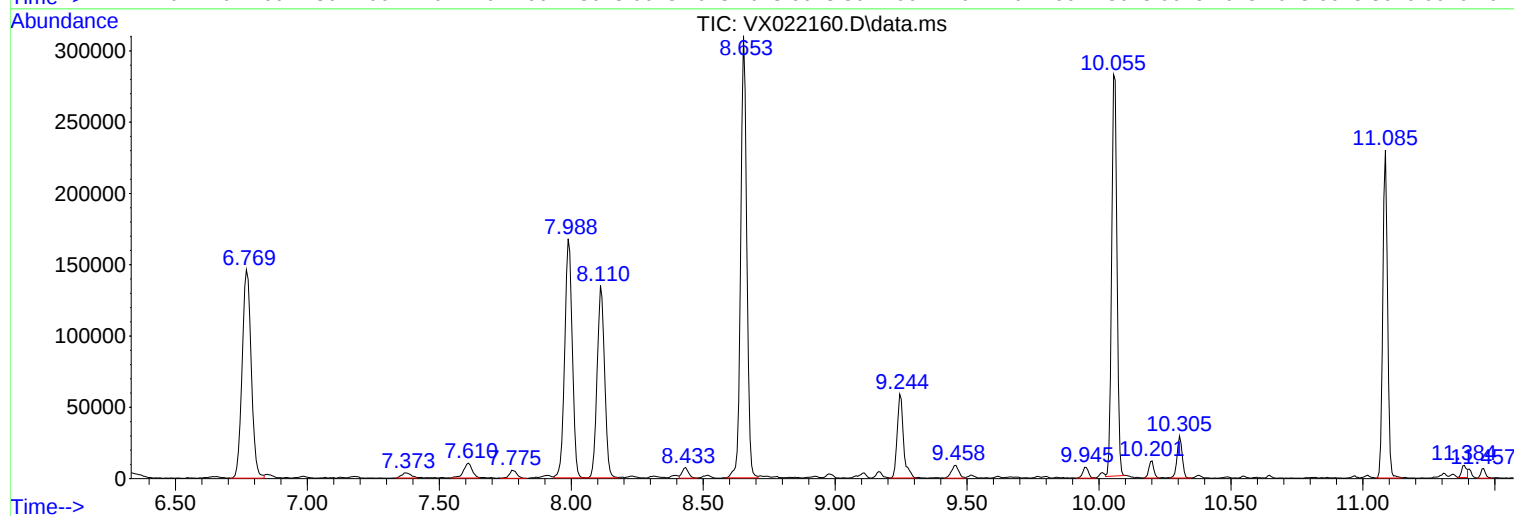
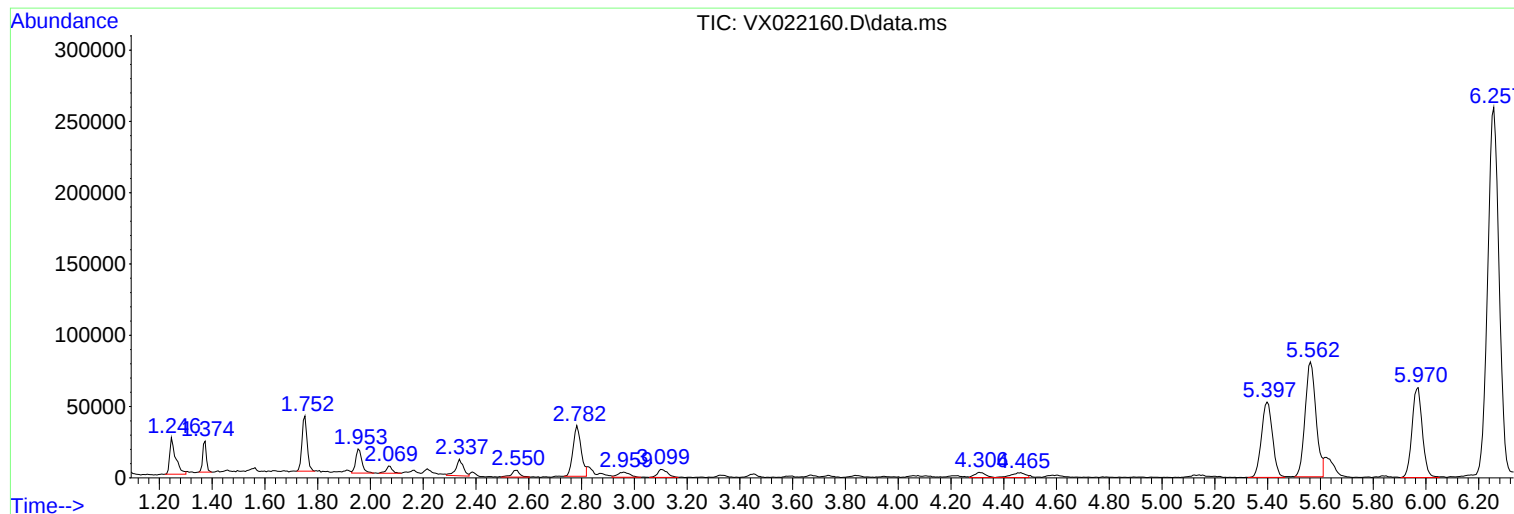
Sum of corrected areas: 4598324

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052421\
Data File : VX022160.D
Acq On : 24 May 2021 20:08
Operator : JC/MD
Sample : M2504-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052421\
Data File : VX022160.D
Acq On : 24 May 2021 20:08
Operator : JC/MD
Sample : M2504-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

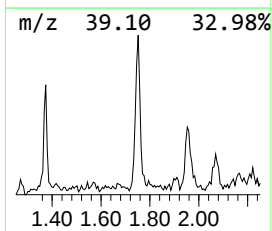
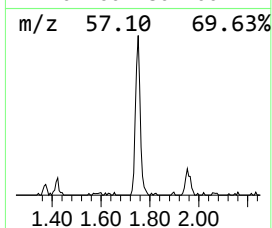
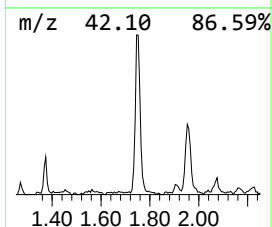
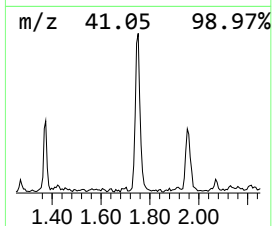
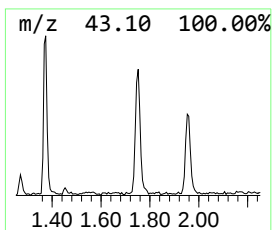
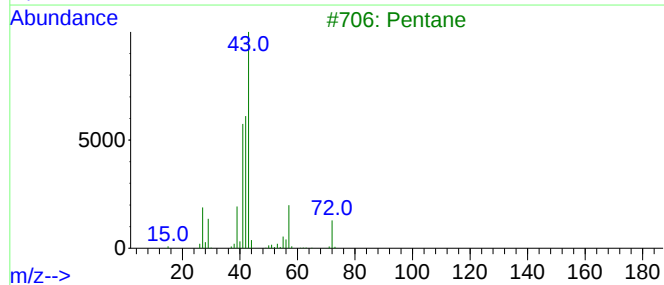
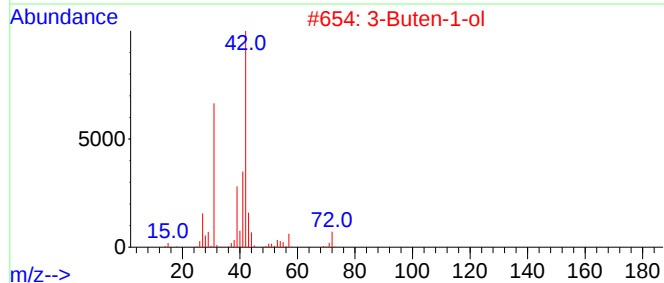
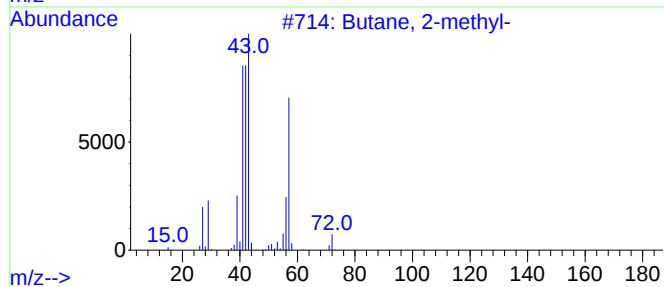
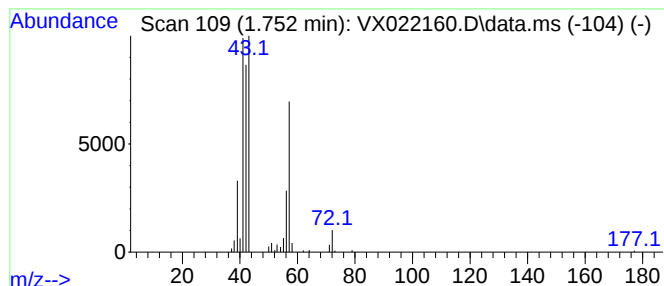
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	11.18 ug/l	52415	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	91
2			3-Buten-1-ol	72	C4H8O	000627-27-0	47
3			Pentane	72	C5H12	000109-66-0	33
4			1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	33
5			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	16



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052421\
Data File : VX022160.D
Acq On : 24 May 2021 20:08
Operator : JC/MD
Sample : M2504-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

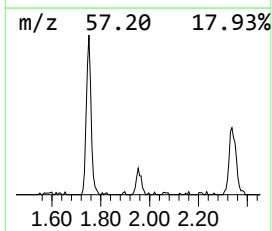
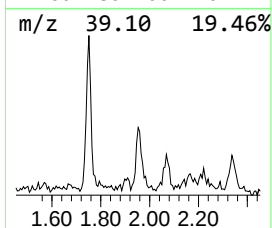
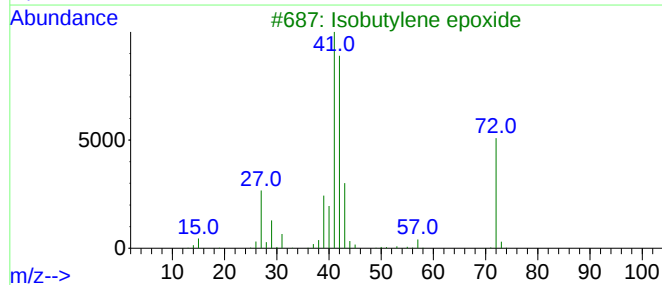
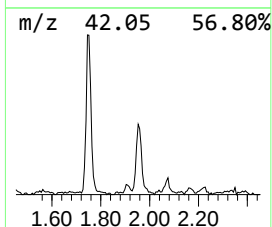
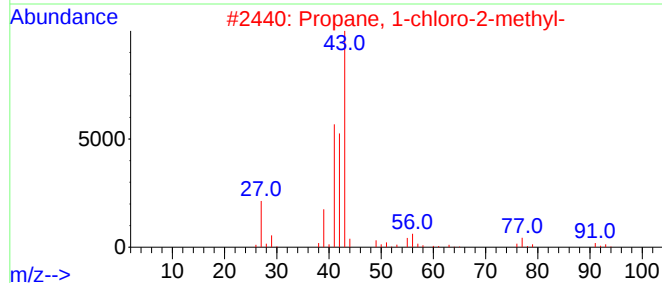
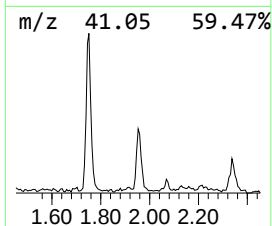
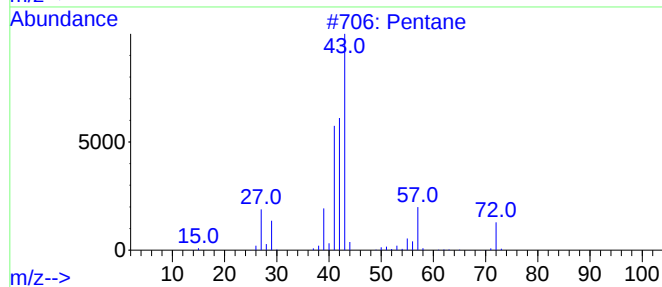
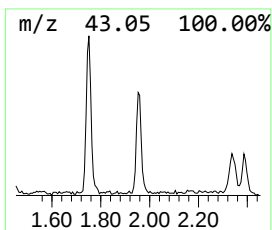
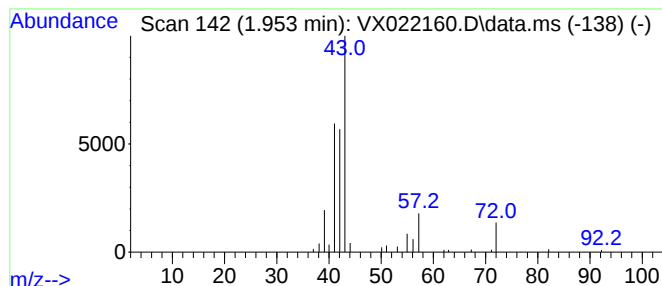
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.953	5.76 ug/l	27005	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	91
2			Propane, 1-chloro-2-methyl-	92	C4H9Cl	000513-36-0	53
3			Isobutylene epoxide	72	C4H8O	000558-30-5	40
4			Oxirane, ethyl-	72	C4H8O	000106-88-7	40
5			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	39



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052421\
Data File : VX022160.D
Acq On : 24 May 2021 20:08
Operator : JC/MD
Sample : M2504-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

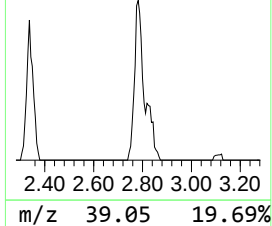
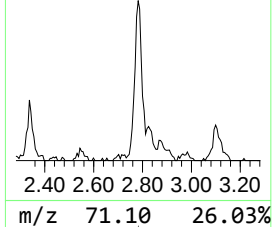
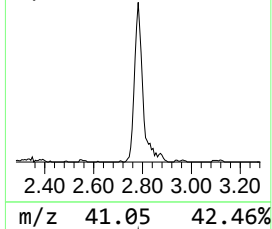
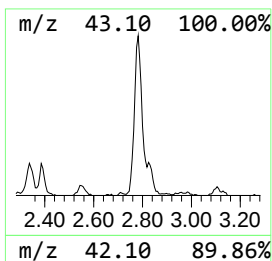
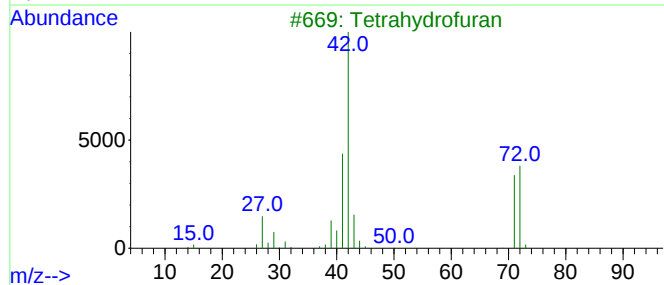
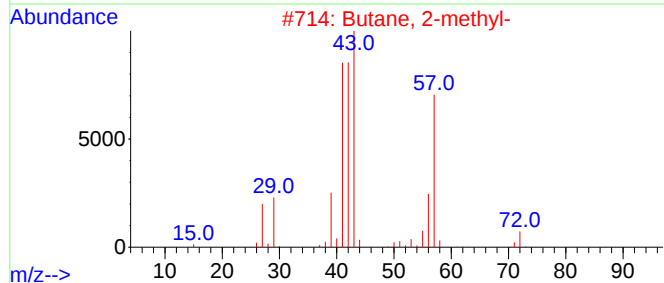
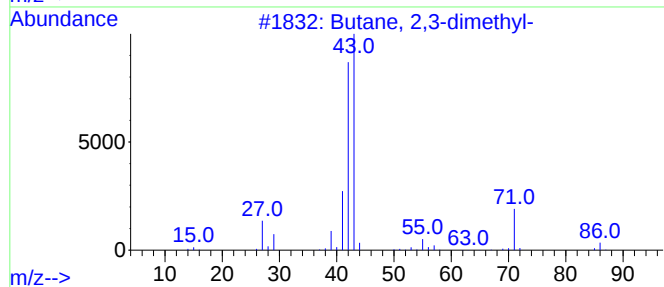
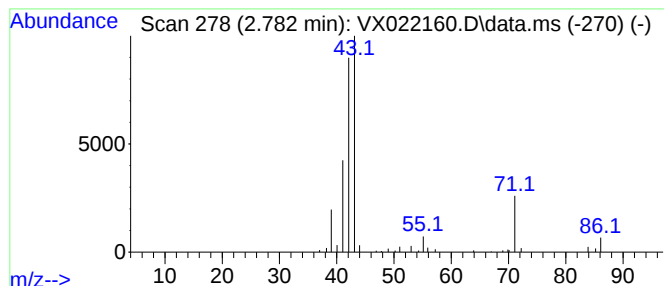
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Butane, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	16.50 ug/l	77342	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
2			Butane, 2-methyl-	72	C5H12	000078-78-4	38
3			Tetrahydrofuran	72	C4H8O	000109-99-9	36
4			Pentane, 2-methyl-	86	C6H14	000107-83-5	33
5			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	14



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052421\
Data File : VX022160.D
Acq On : 24 May 2021 20:08
Operator : JC/MD
Sample : M2504-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

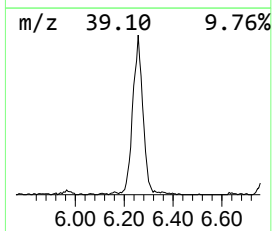
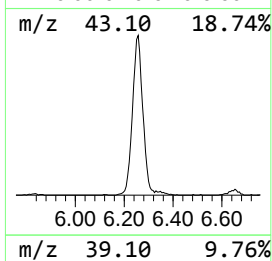
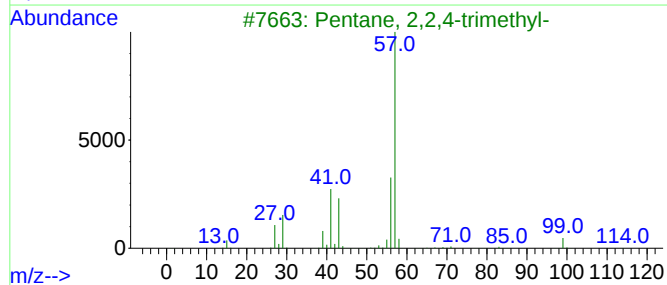
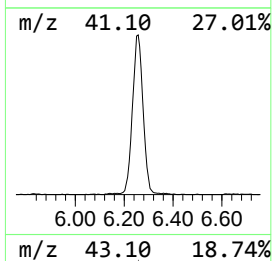
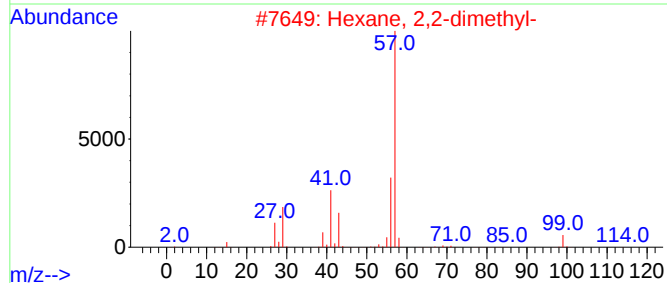
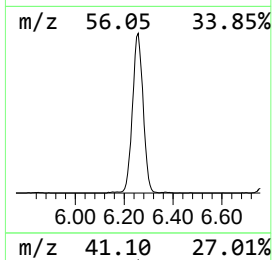
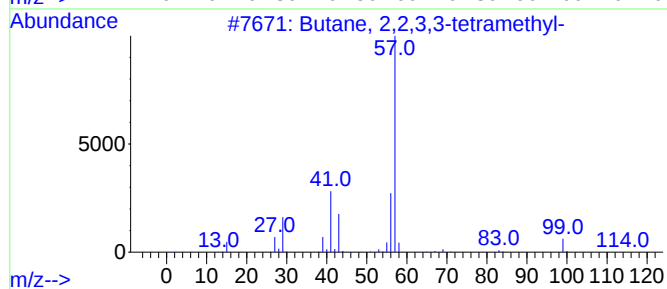
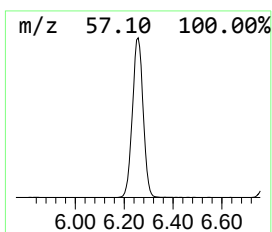
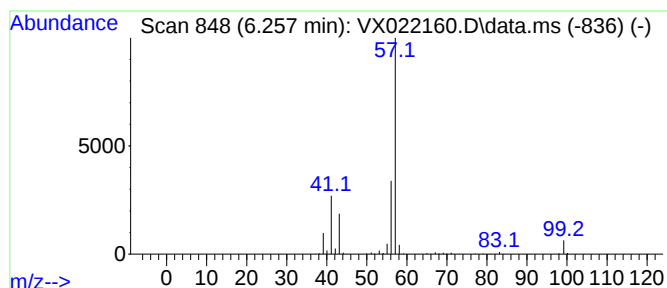
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Butane, 2,2,3,3-tetramethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.257	114.15 ug/l	793065	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
2			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	78
3			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	78
4			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	64
5			Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052421\
Data File : VX022160.D
Acq On : 24 May 2021 20:08
Operator : JC/MD
Sample : M2504-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

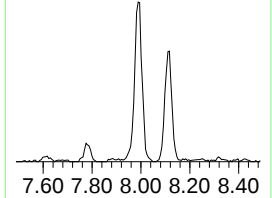
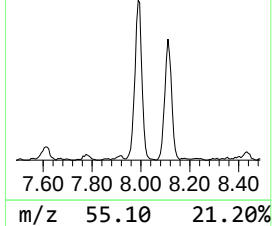
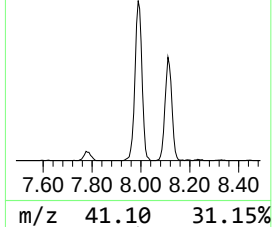
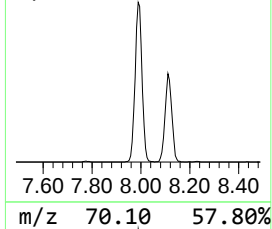
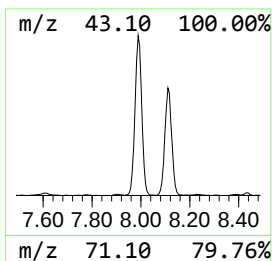
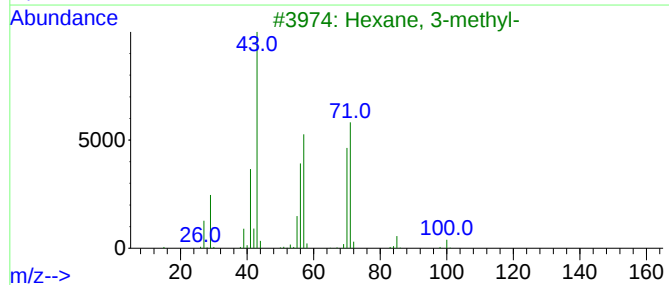
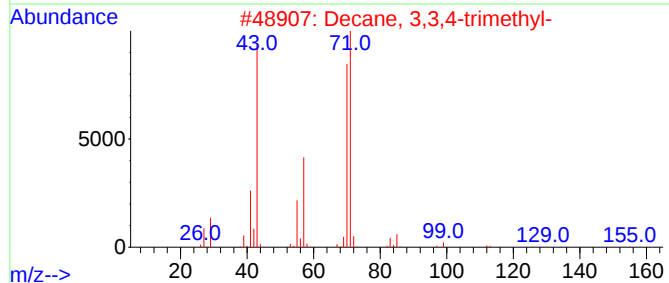
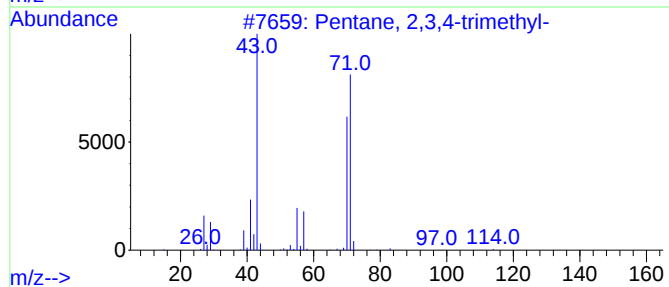
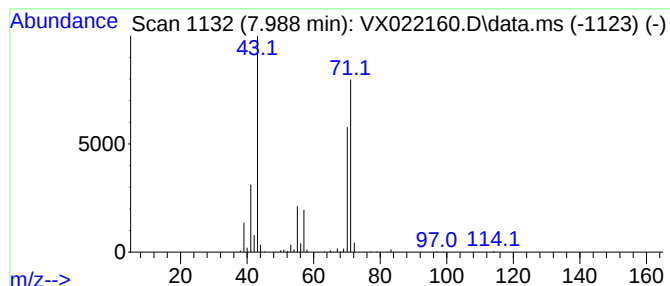
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Pentane, 2,3,4-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.988	47.78 ug/l	331921	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	83
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	78
4			Pentane, 3-ethyl-	100	C7H16	000617-78-7	74
5			Heptane, 4-methyl-	114	C8H18	000589-53-7	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052421\
Data File : VX022160.D
Acq On : 24 May 2021 20:08
Operator : JC/MD
Sample : M2504-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

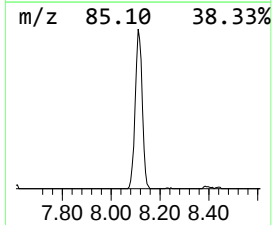
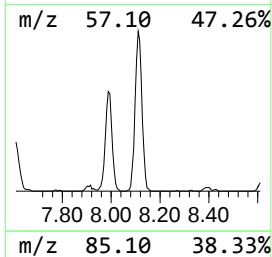
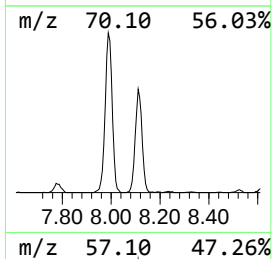
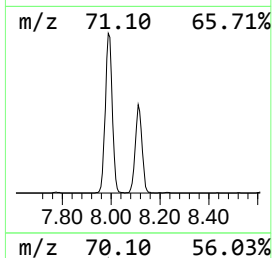
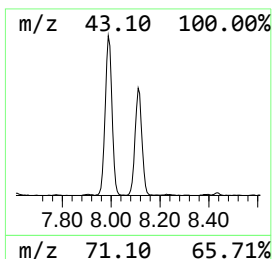
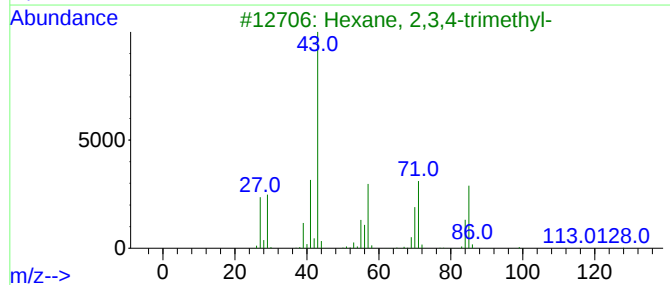
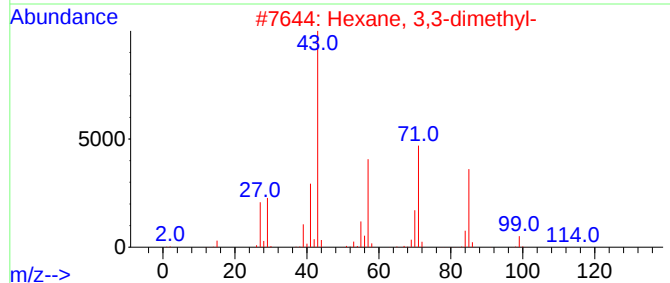
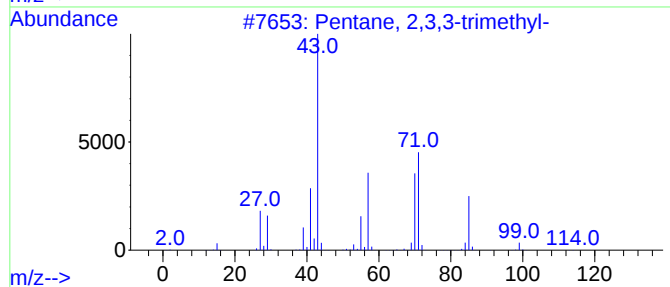
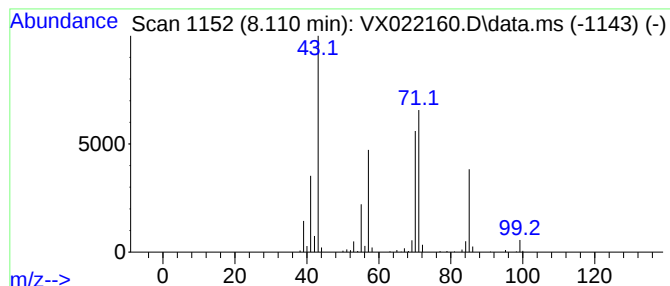
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Pentane, 2,3,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	38.10 ug/l	264716	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
3			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	64
4			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	50
5			Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052421\
Data File : VX022160.D
Acq On : 24 May 2021 20:08
Operator : JC/MD
Sample : M2504-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methyl-	1.752	11.2	ug/l	52415	1	5.562	234335	50.0
Pentane	1.953	5.8	ug/l	27005	1	5.562	234335	50.0
Butane, 2,3-dim...	2.782	16.5	ug/l	77342	1	5.562	234335	50.0
Butane, 2,2,3,3...	6.257	114.2	ug/l	793065	2	6.769	347378	50.0
Pentane, 2,3,4-...	7.988	47.8	ug/l	331921	2	6.769	347378	50.0
Pentane, 2,3,3-...	8.110	38.1	ug/l	264716	2	6.769	347378	50.0