

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121321\
 Data File : VN070055.D
 Acq On : 14 Dec 2021 2:15
 Operator : JC/MD
 Sample : M5007-11
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TOLL-MW-10

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_N\methods\82N120221W.M
 Title : SW846 8260

Signal : TIC: VN070055.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.271	86	105	136	rBV4	189288	545691	6.75%	1.114%
2	2.448	162	171	186	rVB2	213510	346425	4.28%	0.707%
3	5.624	1327	1355	1382	rBV3	101514	369061	4.56%	0.753%
4	7.048	1862	1886	1907	rBV3	64541	188519	2.33%	0.385%
5	7.327	1970	1990	2014	rBV2	155109	417942	5.17%	0.853%
6	8.024	2228	2250	2261	rBV	891711	2145309	26.52%	4.380%
7	8.086	2261	2273	2291	rVV	1452566	3342588	41.32%	6.824%
8	8.174	2292	2306	2326	rVB3	345984	865616	10.70%	1.767%
9	8.440	2385	2405	2435	rBV	1000699	2373315	29.34%	4.845%
10	8.617	2452	2471	2493	rVB	516922	1253692	15.50%	2.559%
11	8.968	2582	2602	2627	rBV	2529755	5239334	64.77%	10.696%
12	9.456	2754	2784	2795	rBV5	64291	200179	2.47%	0.409%
13	9.512	2796	2805	2820	rVB5	41713	82087	1.01%	0.168%
14	9.593	2821	2835	2852	rBV2	53670	113923	1.41%	0.233%
15	9.883	2925	2943	2962	rBV	505726	1007581	12.46%	2.057%
16	10.014	2969	2992	3026	rBV	730707	1532003	18.94%	3.128%
17	10.371	3105	3125	3135	rBV3	98537	186000	2.30%	0.380%
18	10.440	3135	3151	3191	rVB	4157295	7754907	95.87%	15.831%
19	10.642	3218	3226	3242	rVB3	62387	115415	1.43%	0.236%
20	10.717	3242	3254	3267	rVB3	57189	106526	1.32%	0.217%
21	10.870	3298	3311	3332	rVB3	38683	112596	1.39%	0.230%
22	11.744	3619	3637	3677	rBV	4423115	8088961	100.00%	16.513%
23	12.731	3984	4005	4030	rBV	3346901	6024174	74.47%	12.298%
24	13.675	4339	4357	4384	rBV	3716106	6572383	81.25%	13.417%

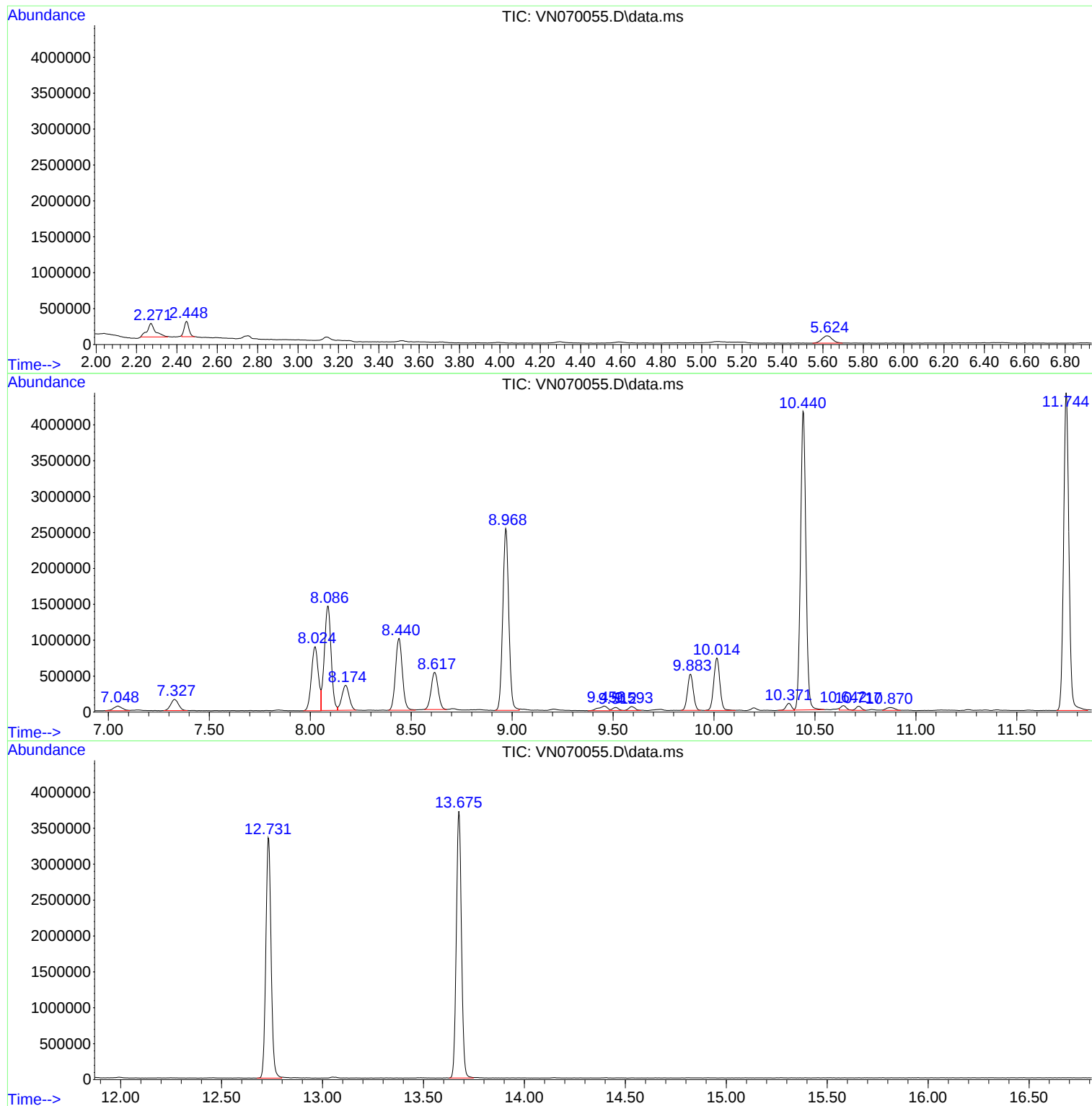
Sum of corrected areas: 48984227

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121321\
Data File : VN070055.D
Acq On : 14 Dec 2021 2:15
Operator : JC/MD
Sample : M5007-11
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-10

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121321\
Data File : VN070055.D
Acq On : 14 Dec 2021 2:15
Operator : JC/MD
Sample : M5007-11
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-10

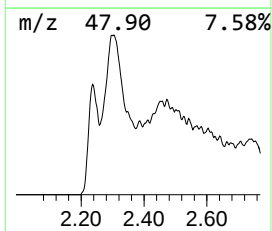
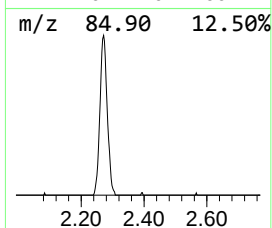
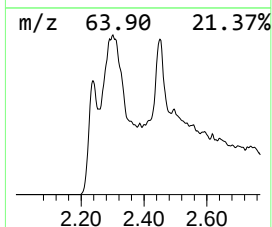
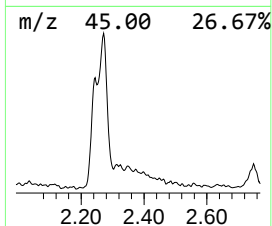
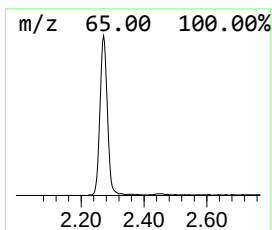
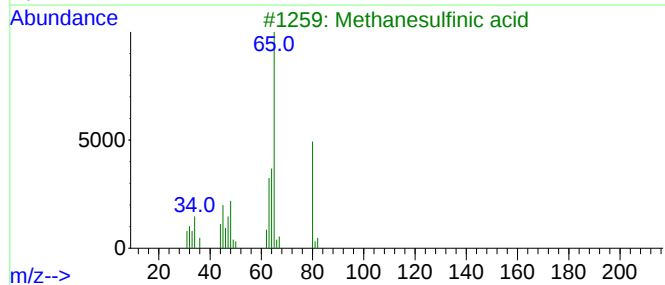
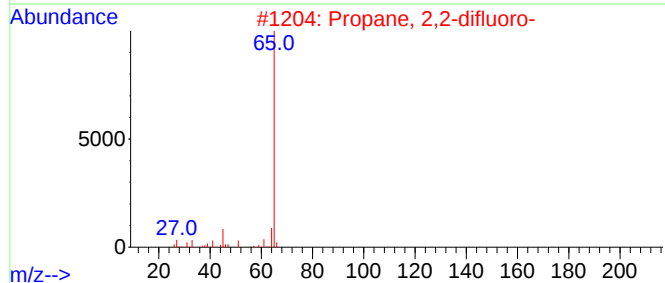
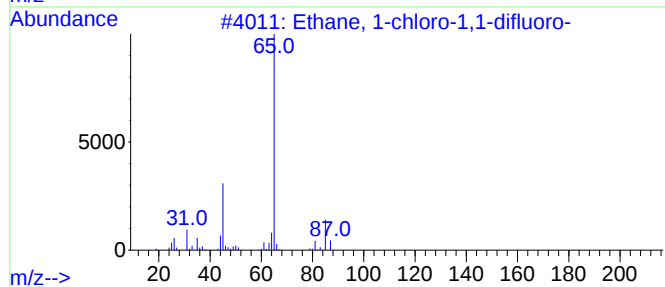
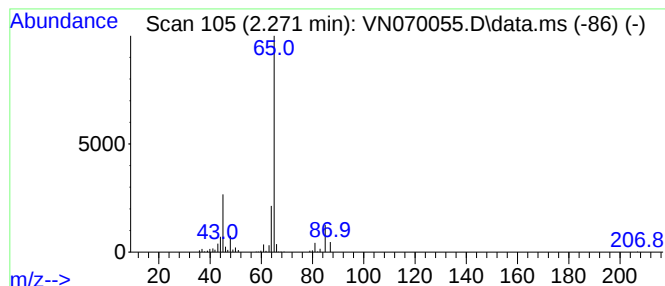
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethane, 1-chloro-1,1-difluoro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.271	8.16 ug/l	545691	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1-chloro-1,1-difluoro-	100	C2H3ClF2	000075-68-3	83
2			Propane, 2,2-difluoro-	80	C3H6F2	000420-45-1	4
3			Methanesulfinic acid	80	CH4O2S	017696-73-0	2
4			2,2-Difluoropropionic acid	110	C3H4F2O2	000373-96-6	2
5			1,2-Difluoroethane	66	C2H4F2	000624-72-6	1



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121321\
Data File : VN070055.D
Acq On : 14 Dec 2021 2:15
Operator : JC/MD
Sample : M5007-11
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-10

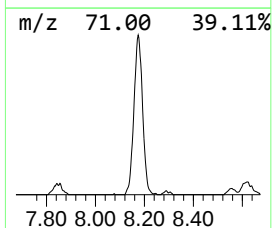
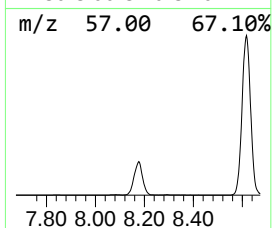
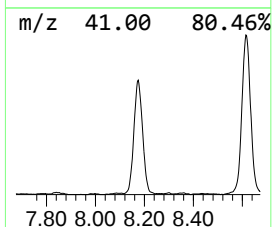
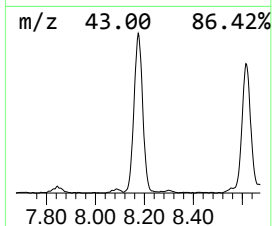
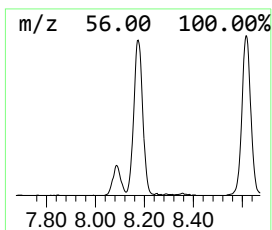
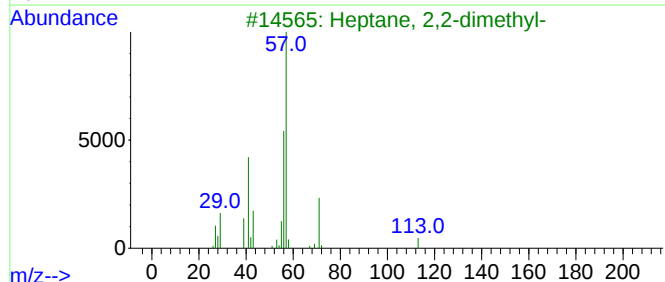
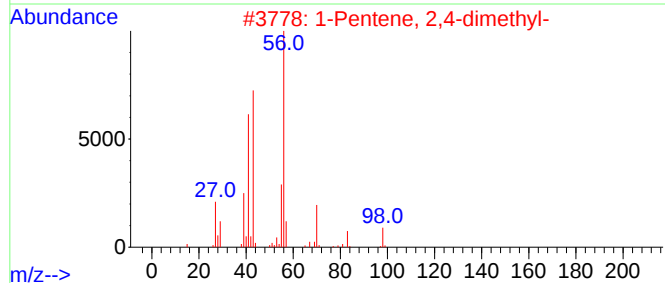
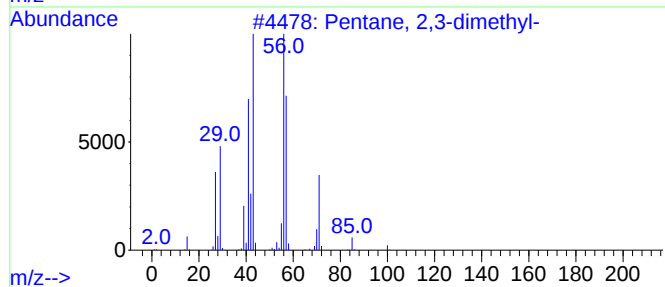
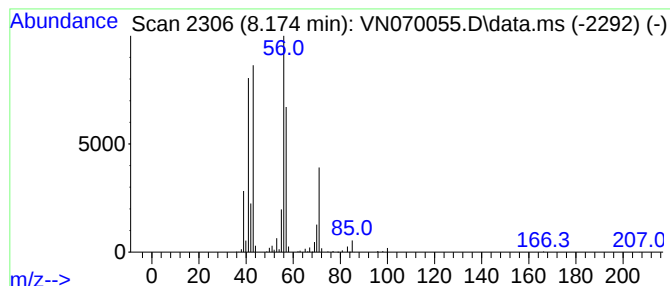
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane, 2,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.174	12.95 ug/l	865616	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2			1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	53
3			Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	42
4			Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	38
5			Cyclopentane, methyl-	84	C6H12	000096-37-7	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121321\
Data File : VN070055.D
Acq On : 14 Dec 2021 2:15
Operator : JC/MD
Sample : M5007-11
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-10

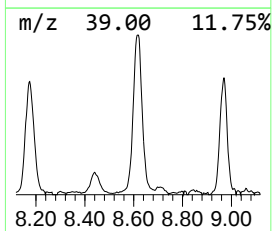
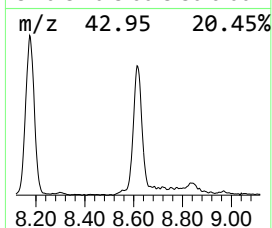
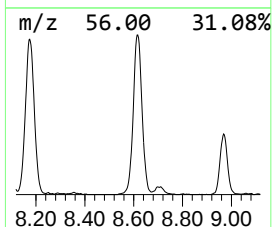
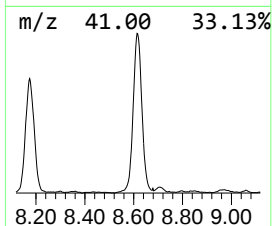
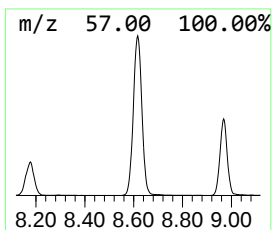
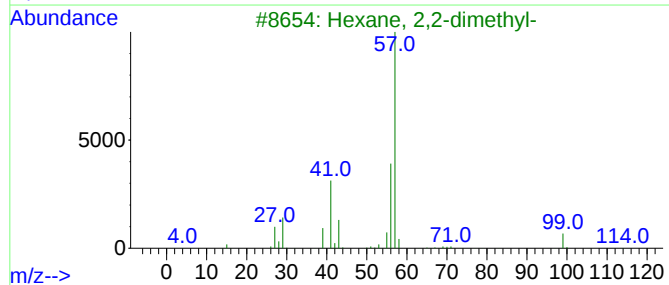
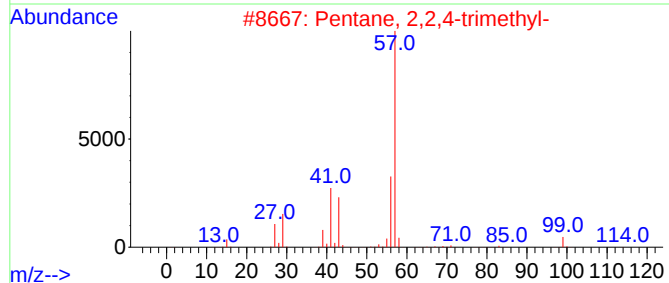
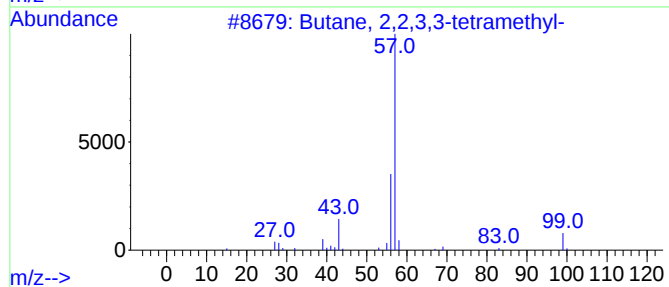
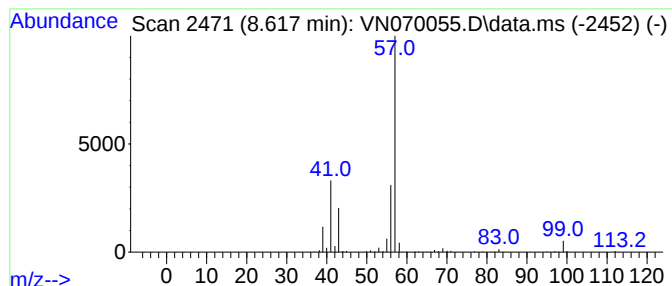
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.617	11.96 ug/l	1253690	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
2			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
3			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
4			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59
5			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121321\
Data File : VN070055.D
Acq On : 14 Dec 2021 2:15
Operator : JC/MD
Sample : M5007-11
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-10

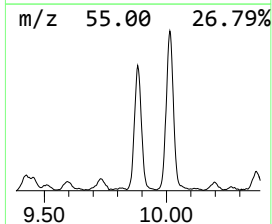
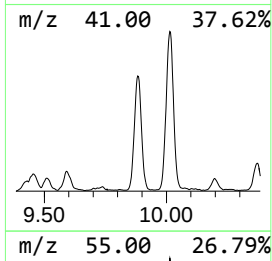
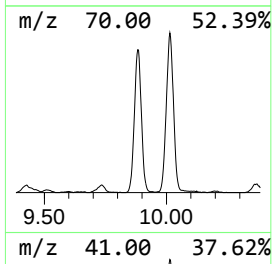
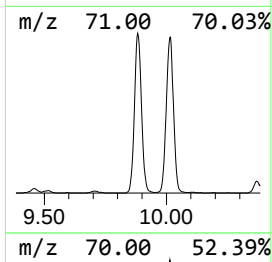
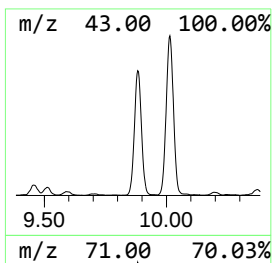
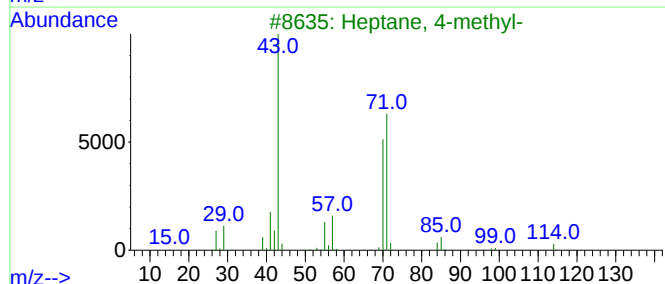
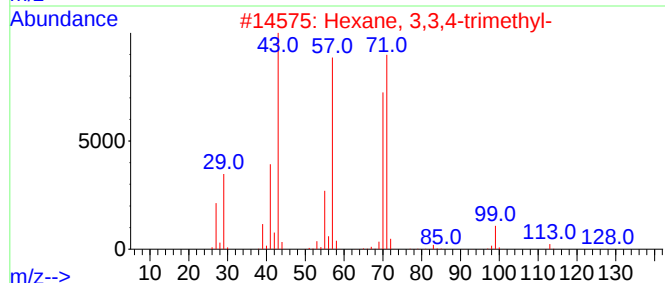
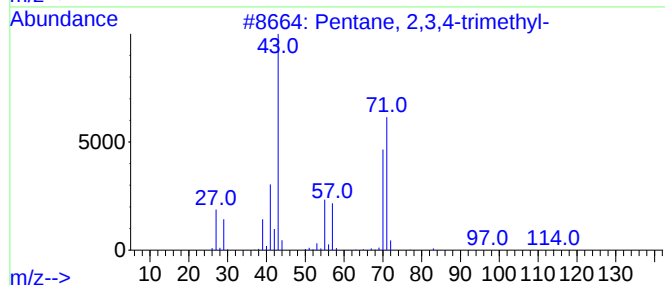
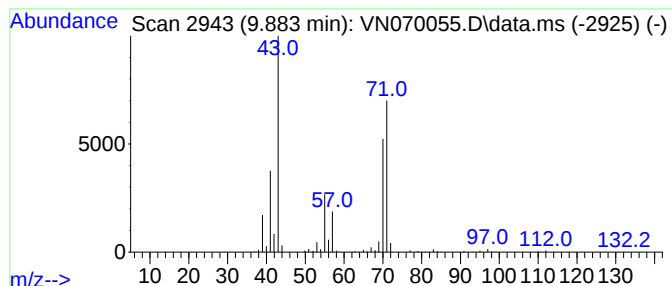
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.883	9.62 ug/l	1007580	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	83
2			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	64
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
4			Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	56
5			1-Butanol, 2,2-dimethyl-	102	C6H14O	001185-33-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121321\
Data File : VN070055.D
Acq On : 14 Dec 2021 2:15
Operator : JC/MD
Sample : M5007-11
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-10

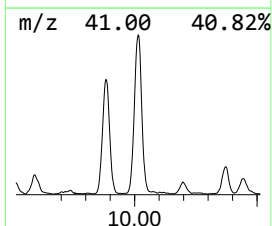
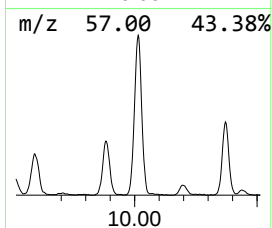
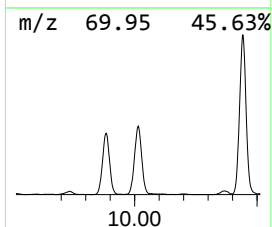
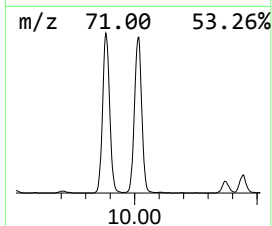
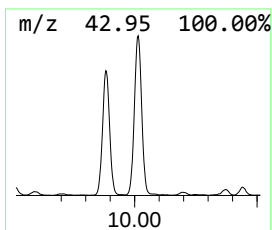
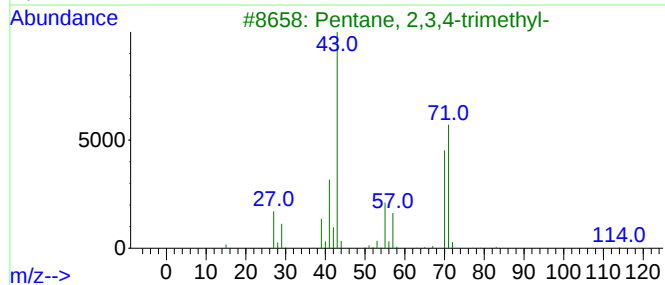
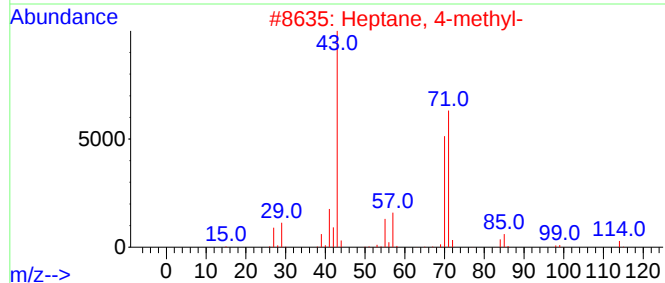
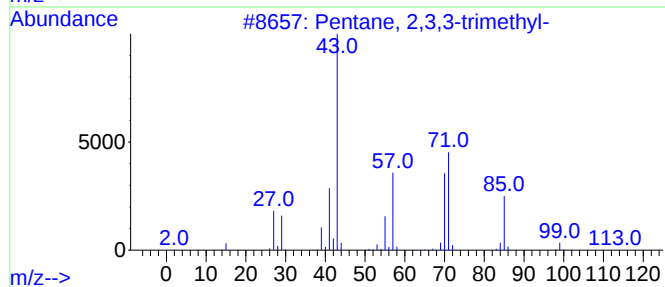
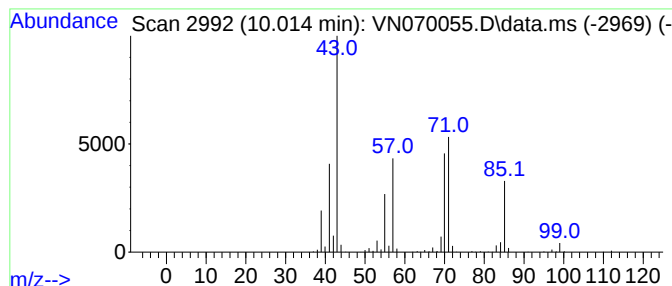
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 5 Pentane, 2,3,3-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.014	14.62 ug/l	1532000	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59
4			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59
5			Propanoic acid, 2-methyl-, 2-eth...	200	C12H24O2	035061-61-1	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121321\
Data File : VN070055.D
Acq On : 14 Dec 2021 2:15
Operator : JC/MD
Sample : M5007-11
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-10

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.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
Ethane, 1-chlor...	2.271	8.2	ug/l	545691	1	8.088	3342590	50.0
Pentane, 2,3-di...	8.174	12.9	ug/l	865616	1	8.088	3342590	50.0
Butane, 2,2,3,3...	8.617	12.0	ug/l	1253690	2	8.968	5239330	50.0
Pentane, 2,3,4-...	9.883	9.6	ug/l	1007580	2	8.968	5239330	50.0
Pentane, 2,3,3-...	10.014	14.6	ug/l	1532000	2	8.968	5239330	50.0