LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121222\
Data File : VN075726.D
Acq On : 12 Dec 2022 20:29
Operator : JC\MD
Sample : N5978-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 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\82N120922W.M
Title : SW846 8260

Signal : TIC: VN075726.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.301	33	42	45	rBV	22929	52965	4.98%	0.748%
2	2.336	45	48	62	rVB	36818	75379	7.09%	1.064%
3	2.524	75	80	89	rBV	35137	58273	5.48%	0.823%
4	2.824	125	131	139	rVB4	9523	25471	2.39%	0.360%
5	3.248	199	203	211	rVB6	7851	19307	1.82%	0.273%
6	5.812	629	639	653	rBV2	13516	45297	4.26%	0.640%
7	7.235	872	881	892	rVB4	10735	32342	3.04%	0.457%
8	7.494	917	925	936	rVB3	25342	66240	6.23%	0.935%
9	8.177	1030	1041	1045	rBV	147556	359390	33.79%	5.074%
10	8.230	1045	1050	1059	rVV	298671	649095	61.02%	9.165%
11	8.335	1059	1068	1077	rVB2	63984	154894	14.56%	2.187%
12	8.588	1101	1111	1120	rBV	146817	330721	31.09%	4.670%
13	8.765	1131	1141	1151	rVV	119088	281007	26.42%	3.968%
14	9.106	1190	1199	1212	rBV	393577	790994	74.36%	11.168%
15	9.588	1271	1281	1287	rBV5	14713	40270	3.79%	0.569%
16	9.647	1287	1291	1298	rVB5	10895	20680	1.94%	0.292%
17	9.735	1299	1306	1313	rBV2	12866	26187	2.46%	0.370%
18	10.018	1345	1354	1365	rBV2	125408	243667	22.91%	3.440%
19	10.153	1365	1377	1386	rBV	175411	359805	33.82%	5.080%
20	10.329	1401	1407	1413	rBV3	8165	15115	1.42%	0.213%
21	10.494	1429	1435	1441	rBV	26832	48323	4.54%	0.682%
22	10.571	1441	1448	1462	rVB	585256	1063731	100.00%	15.019%
23	10.765	1473	1481	1488	rVB3	15022	30192	2.84%	0.426%
24	10.835	1488	1493	1500	rVB3	11970	21701	2.04%	0.306%
25	11.006	1513	1522	1530	rVB7	11401	33545	3.15%	0.474%
26	11.870	1661	1669	1676	rBV	487381	877690	82.51%	12.392%
27	12.853	1829	1836	1845	rBV	374964	628778	59.11%	8.878%
28	13.794	1989	1996	2008	rBV	445707	731425	68.76%	10.327%

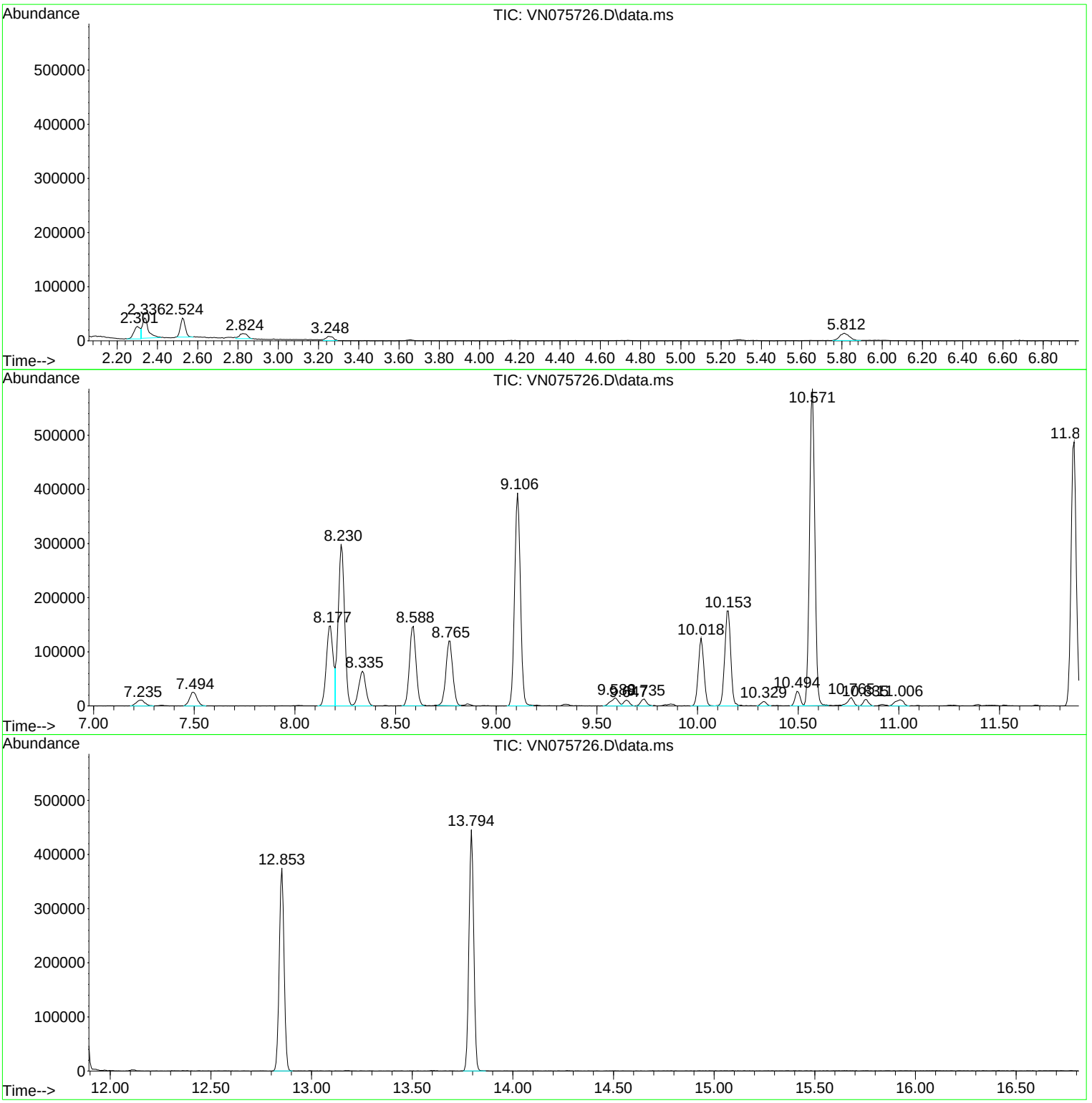
Sum of corrected areas: 7082484

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121222\
Data File : VN075726.D
Acq On : 12 Dec 2022 20:29
Operator : JC\MD
Sample : N5978-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-10

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120922W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121222\
Data File : VN075726.D
Acq On : 12 Dec 2022 20:29
Operator : JC\MD
Sample : N5978-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-10

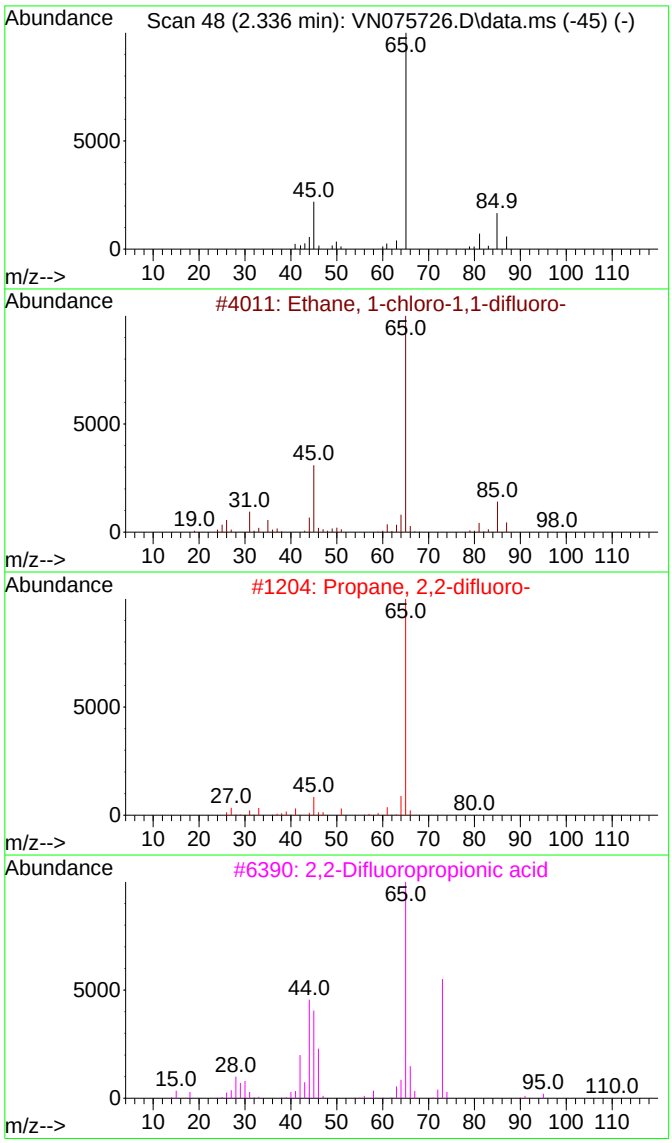
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120922W.M
Quant Title : SW846 8260

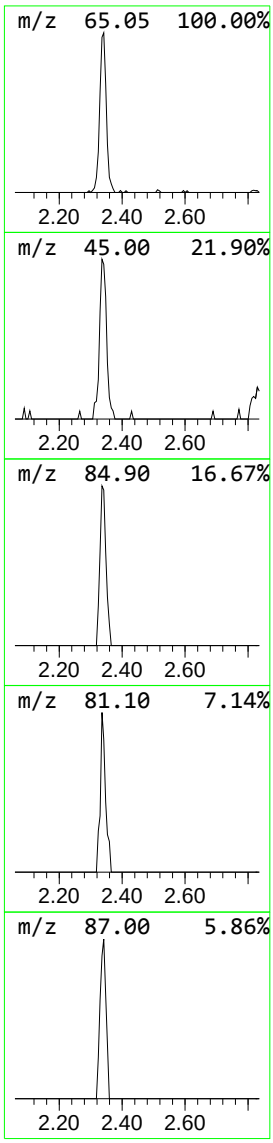
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.336	5.81 ug/l	75379	Pentafluorobenzene	8.230

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	2
3	2,2-Difluoropropionic acid	110	C3H4F2O2	000373-96-6	1
4	Methanesulfinic acid	80	CH4O2S	017696-73-0	1
5	Ethanesulfonyl fluoride	112	C2H5FO2S	000754-03-0	1





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121222\
Data File : VN075726.D
Acq On : 12 Dec 2022 20:29
Operator : JC\MD
Sample : N5978-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-10

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120922W.M
Quant Title : SW846 8260

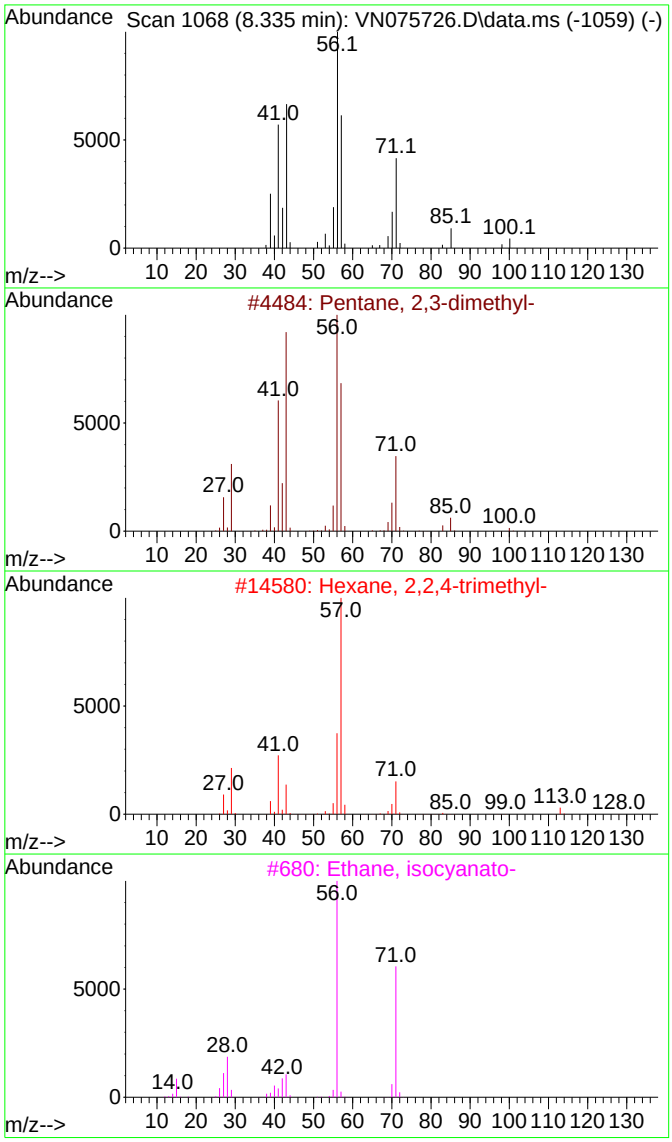
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

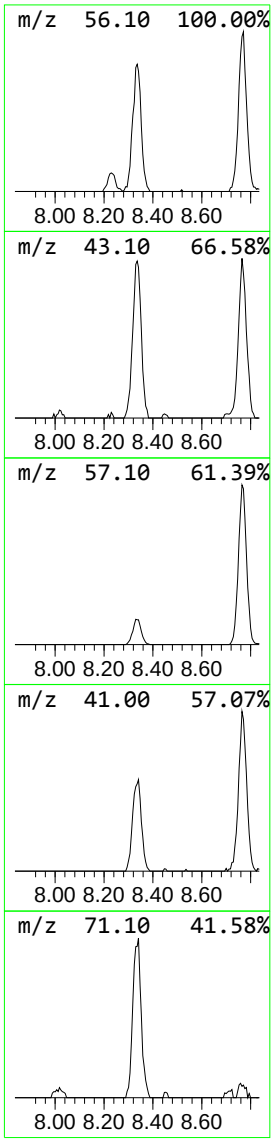
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.335	11.93 ug/l	154894	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	83
2	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	64
3	Ethane, isocyanato-	71	C3H5NO	000109-90-0	50
4	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	47
5	Aziridine, 2-methyl-	57	C3H7N	000075-55-8	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121222\
Data File : VN075726.D
Acq On : 12 Dec 2022 20:29
Operator : JC\MD
Sample : N5978-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-10

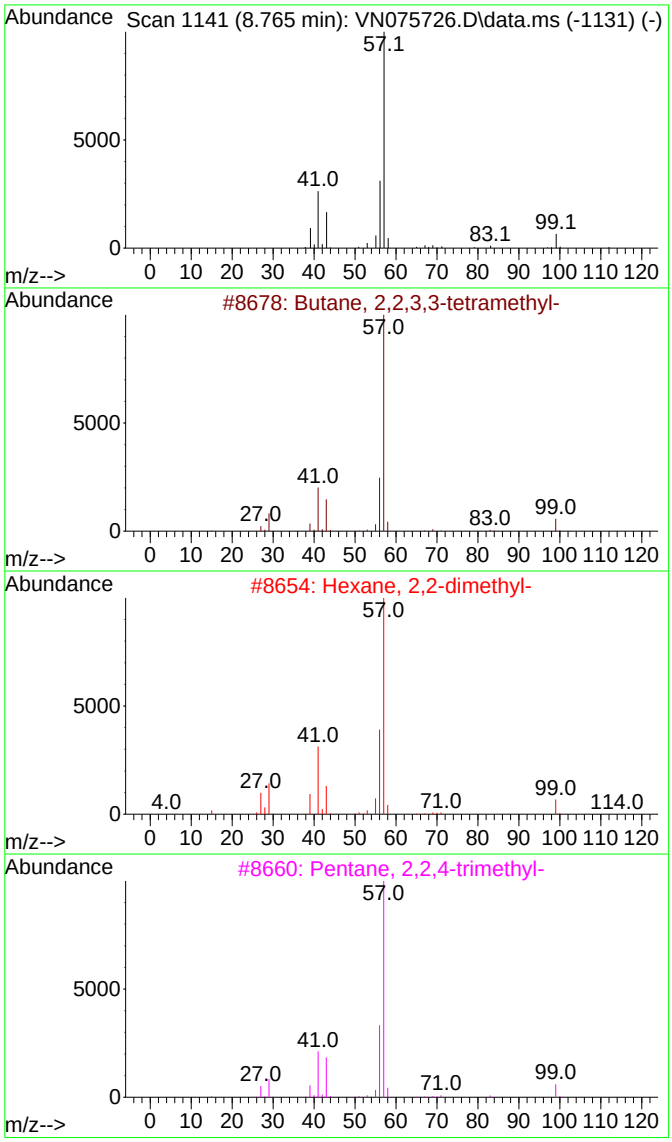
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120922W.M
Quant Title : SW846 8260

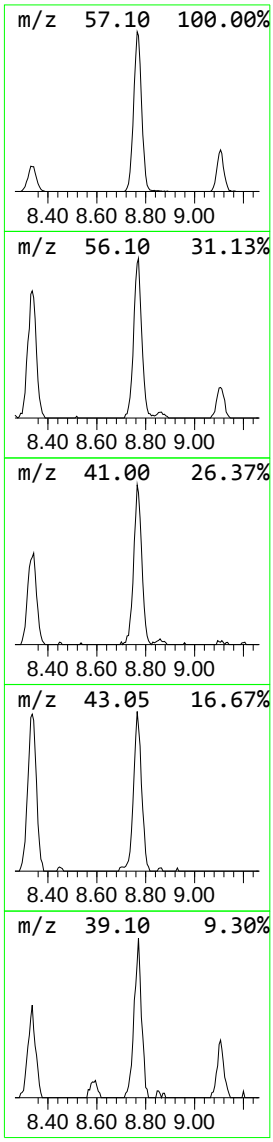
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.765	17.76 ug/l	281007	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
2	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
3	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	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	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121222\
Data File : VN075726.D
Acq On : 12 Dec 2022 20:29
Operator : JC\MD
Sample : N5978-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-10

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120922W.M
Quant Title : SW846 8260

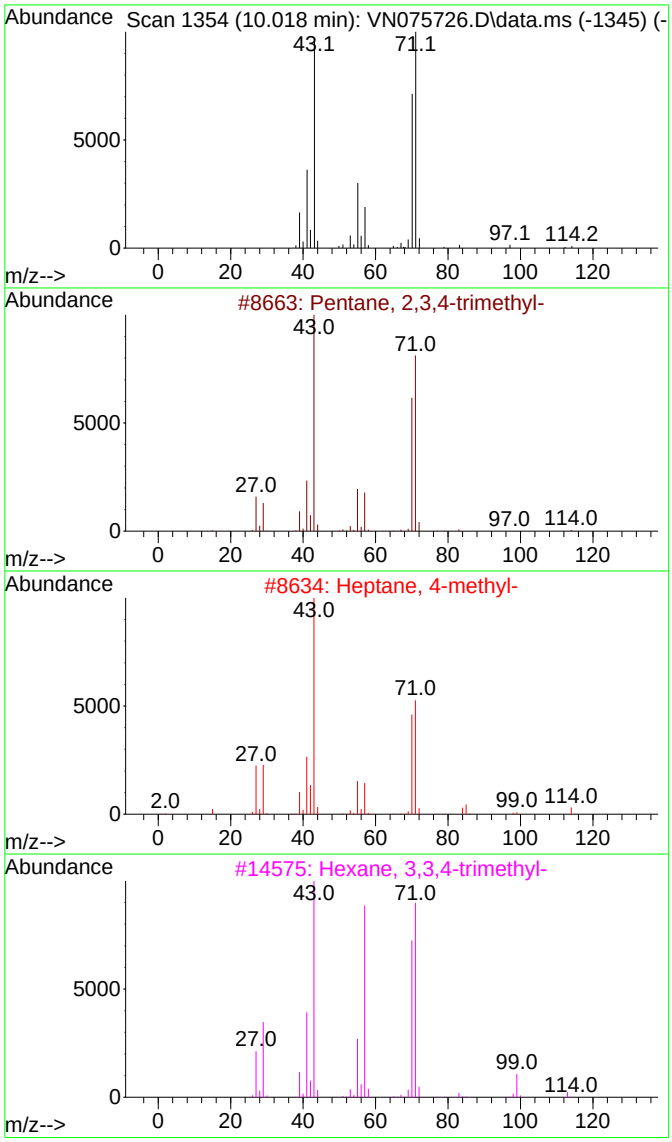
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

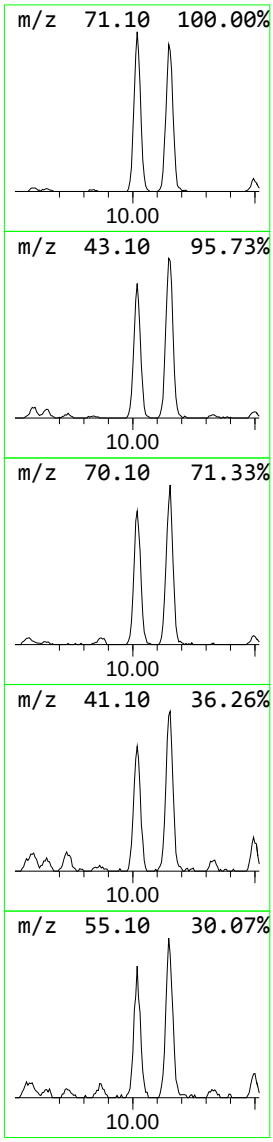
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.018	15.40 ug/l	243667	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	90
2	Heptane, 4-methyl-	114	C8H18	000589-53-7	90
3	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	83
4	Pentane, 3-ethyl-	100	C7H16	000617-78-7	74
5	Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121222\
Data File : VN075726.D
Acq On : 12 Dec 2022 20:29
Operator : JC\MD
Sample : N5978-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-10

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120922W.M
Quant Title : SW846 8260

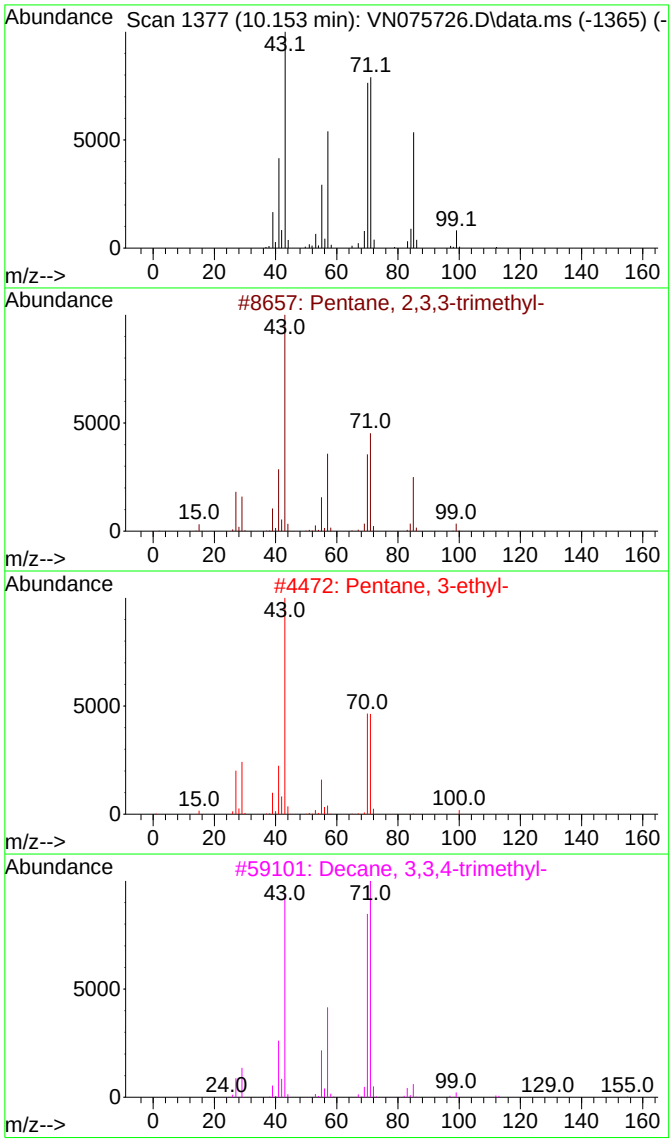
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

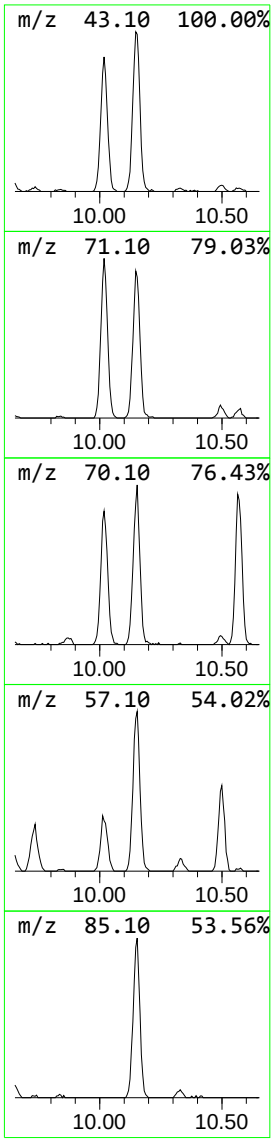
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.153	22.74 ug/l	359805	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	78
2	Pentane, 3-ethyl-	100	C7H16	000617-78-7	64
3	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	64
4	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	64
5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121222\
Data File : VN075726.D
Acq On : 12 Dec 2022 20:29
Operator : JC\MD
Sample : N5978-11
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-10

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120922W.M
Quant Title : SW846 8260

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethane, 1-chlor...	2.336	5.8	ug/l	75379	1	8.230	649095	50.0
Pentane, 2,3-di...	8.335	11.9	ug/l	154894	1	8.230	649095	50.0
Butane, 2,2,3,3...	8.765	17.8	ug/l	281007	2	9.106	790994	50.0
Pentane, 2,3,4-...	10.018	15.4	ug/l	243667	2	9.106	790994	50.0
Pentane, 2,3,3-...	10.153	22.7	ug/l	359805	2	9.106	790994	50.0