LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN101520\
Data File : VN064154.D
Acq On : 15 Oct 2020 19:31
Operator : JC/MD
Sample : L4417-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_N
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_N\METHODS\82N101420W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.415	200	210	219	rBV2	32732	55323	3.11%	0.522%
2	2.779	307	323	338	rBV2	127617	269054	15.11%	2.540%
3	3.107	413	425	436	rBV4	13530	30357	1.71%	0.287%
4	3.766	606	630	652	rBV5	80163	259401	14.57%	2.448%
5	4.486	831	854	855	rBV3	71248	138777	7.79%	1.310%
6	5.004	992	1015	1035	rBV4	28995	108689	6.10%	1.026%
7	6.476	1457	1473	1490	rVB4	19097	57849	3.25%	0.546%
8	7.550	1787	1807	1819	rBV2	233642	596976	33.53%	5.635%
9	7.627	1819	1831	1846	rVV	348227	850303	47.76%	8.026%
10	7.708	1846	1856	1872	rVB3	34368	90586	5.09%	0.855%
11	7.991	1927	1944	1965	rBV	247778	593831	33.35%	5.605%
12	8.174	1989	2001	2018	rVB2	74747	196174	11.02%	1.852%
13	8.550	2102	2118	2143	rBV	584966	1258193	70.67%	11.876%
14	9.489	2396	2410	2422	rBV3	42787	86188	4.84%	0.814%
15	9.621	2435	2451	2466	rBV2	71529	155281	8.72%	1.466%
16	9.991	2554	2566	2573	rBV10	9722	19894	1.12%	0.188%
17	10.061	2573	2588	2606	rVV	979749	1780399	100.00%	16.805%
18	11.380	2984	2998	3019	rBV	929549	1648195	92.57%	15.557%
19	12.379	3295	3309	3334	rBV	657876	1149374	64.56%	10.849%
20	13.318	3587	3601	3622	rBV	716485	1249733	70.19%	11.796%

Sum of corrected areas: 10594577

LSC Report - Integrated Chromatogram

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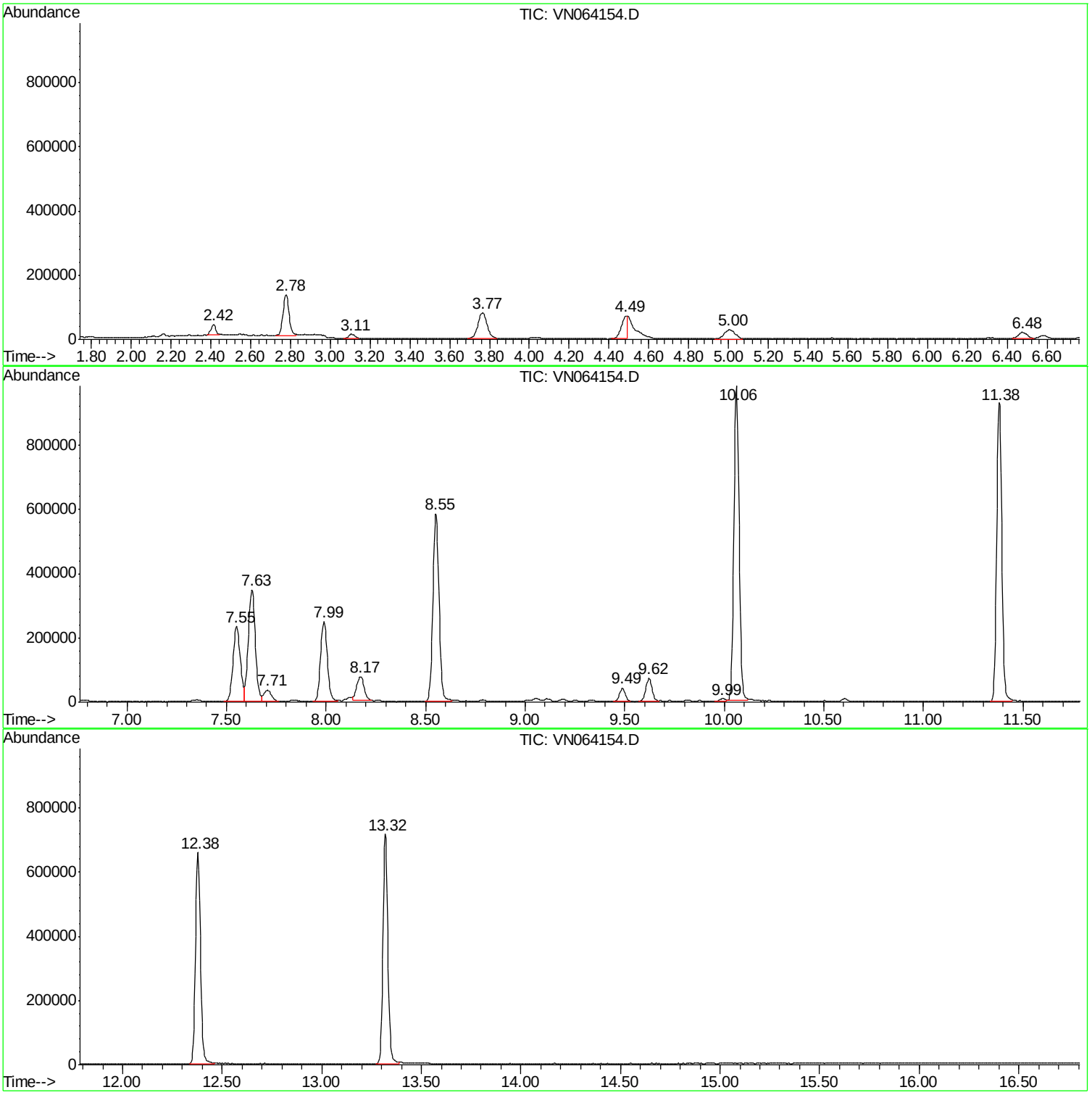
Data File : VN064154.D
Acq On : 15 Oct 2020 19:31
Operator : JC/MD
Sample : L4417-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N101420W.M
Quant Title : SW846 8260

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN101520\
Data File : VN064154.D
Acq On : 15 Oct 2020 19:31
Operator : JC/MD
Sample : L4417-07
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N101420W.M
Quant Title : SW846 8260

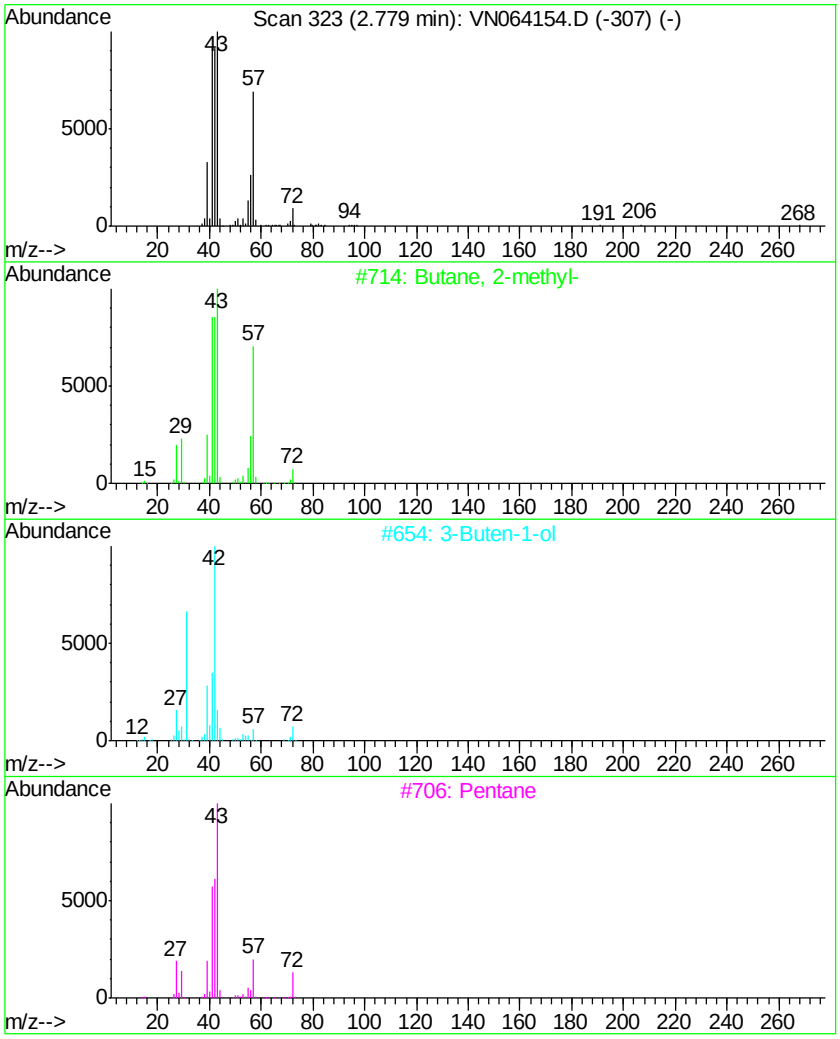
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

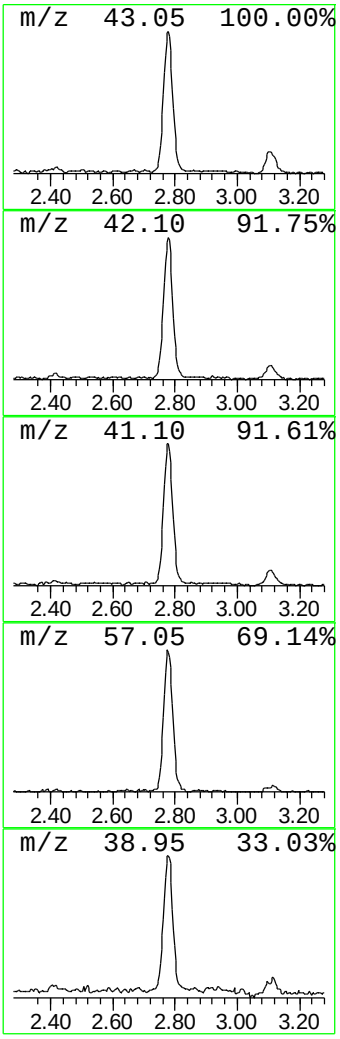
****

Peak Number 1 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.78	15.82 ug/l	269054	Pentafluorobenzene	7.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	94
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47
3	Pentane	72	C5H12	000109-66-0	42
4	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	33
5	Butane, 1-isocyano-	83	C5H9N	002769-64-4	14





Library Search Compound Report

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Data File : VN064154.D
Acq On : 15 Oct 2020 19:31
Operator : JC/MD
Sample : L4417-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N101420W.M
Quant Title : SW846 8260

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

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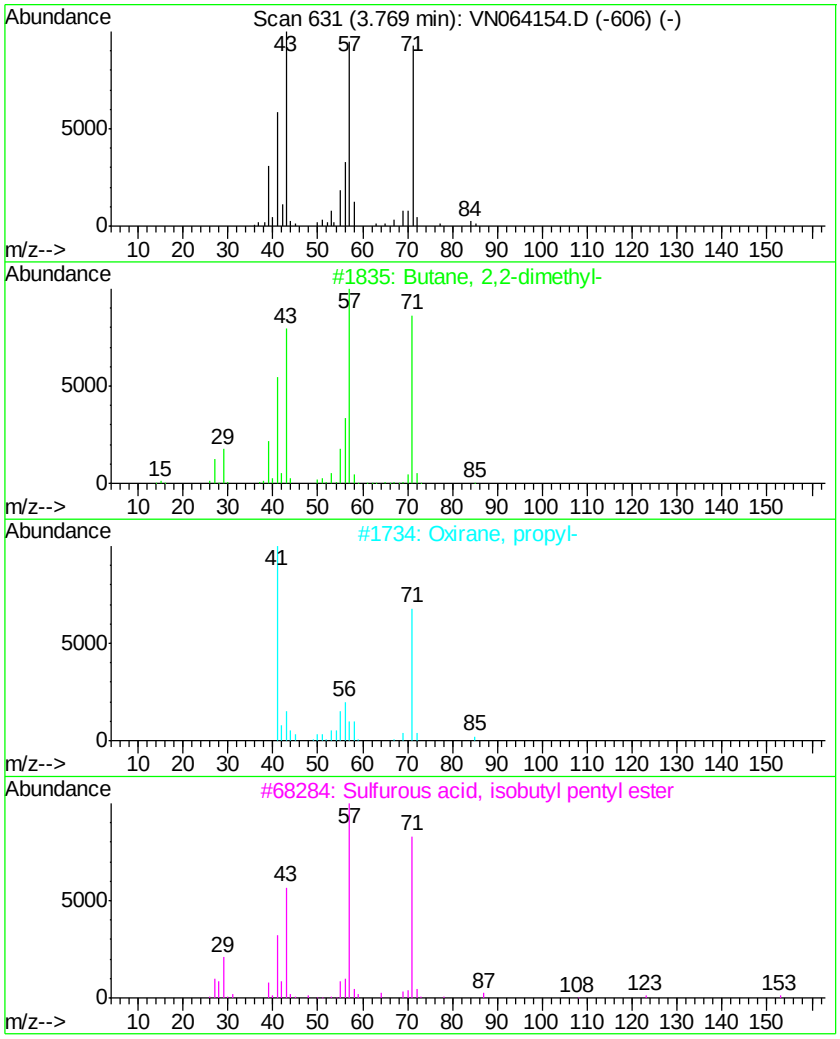
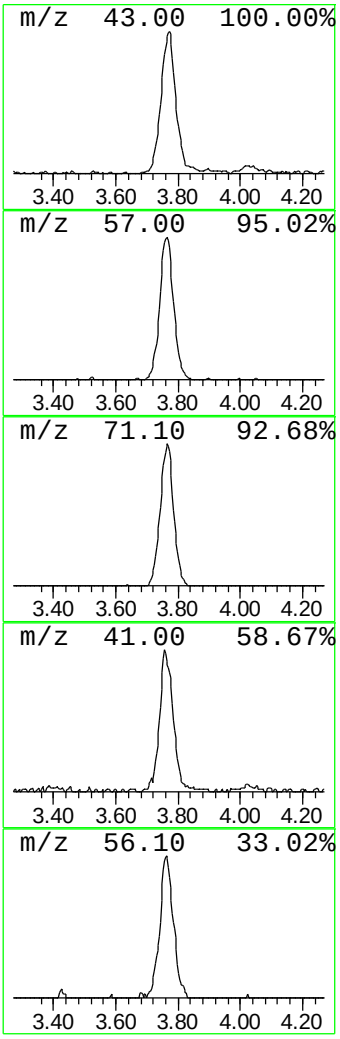
Peak Number 2 Butane, 2,2-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.77	15.25 ug/l	259401	Pentafluorobenzene	7.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	86
2	Oxirane, propyl-	86	C5H10O	001003-14-1	59
3	Sulfurous acid, isobutyl pentyl ...	208	C9H20O3S	1000309-13-8	56
4	Pentane, 3-bromo-	150	C5H11Br	001809-10-5	40
5	Butane, 2-bromo-2-methyl-	150	C5H11Br	000507-36-8	40





Library Search Compound Report

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Data File : VN064154.D
Acq On : 15 Oct 2020 19:31
Operator : JC/MD
Sample : L4417-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N101420W.M
Quant Title : SW846 8260

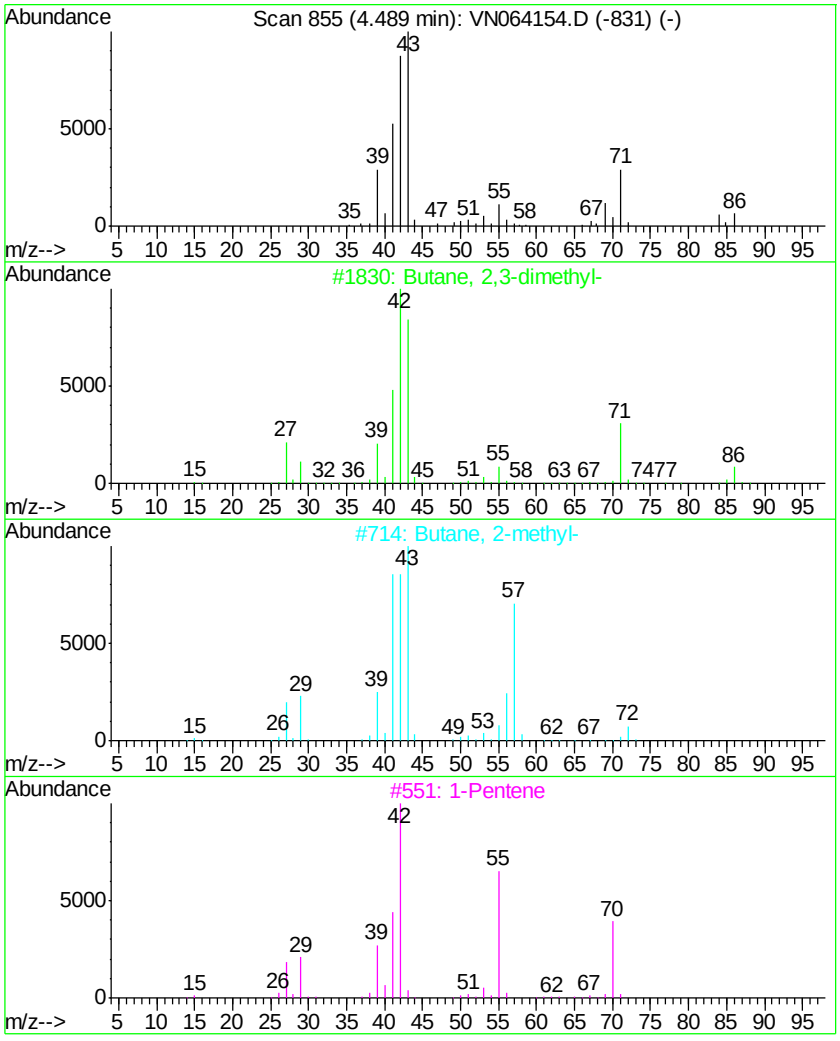
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

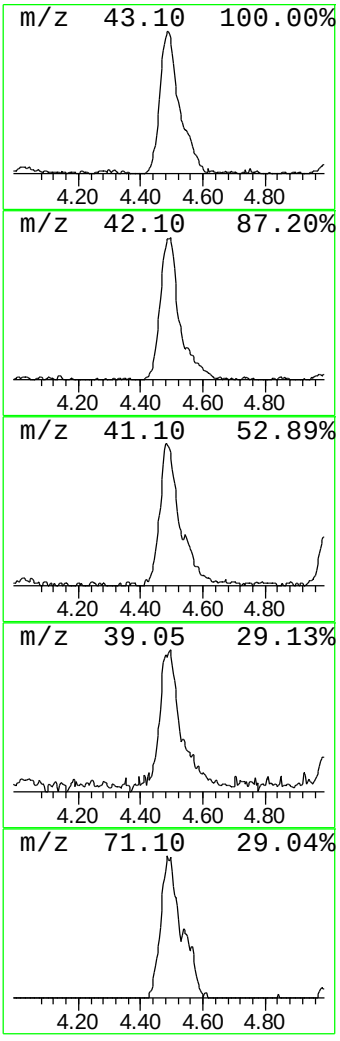
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.49	8.16 ug/l	138777	Pentafluorobenzene	7.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	59
2	Butane, 2-methyl-	72	C5H12	000078-78-4	33
3	1-Pentene	70	C5H10	000109-67-1	28
4	Oxalic acid, allyl octyl ester	242	C13H22O4	1000309-23-6	12
5	Pentane, 2-bromo-	150	C5H11Br	000107-81-3	12





Library Search Compound Report

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Data File : VN064154.D
Acq On : 15 Oct 2020 19:31
Operator : JC/MD
Sample : L4417-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N101420W.M
Quant Title : SW846 8260

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

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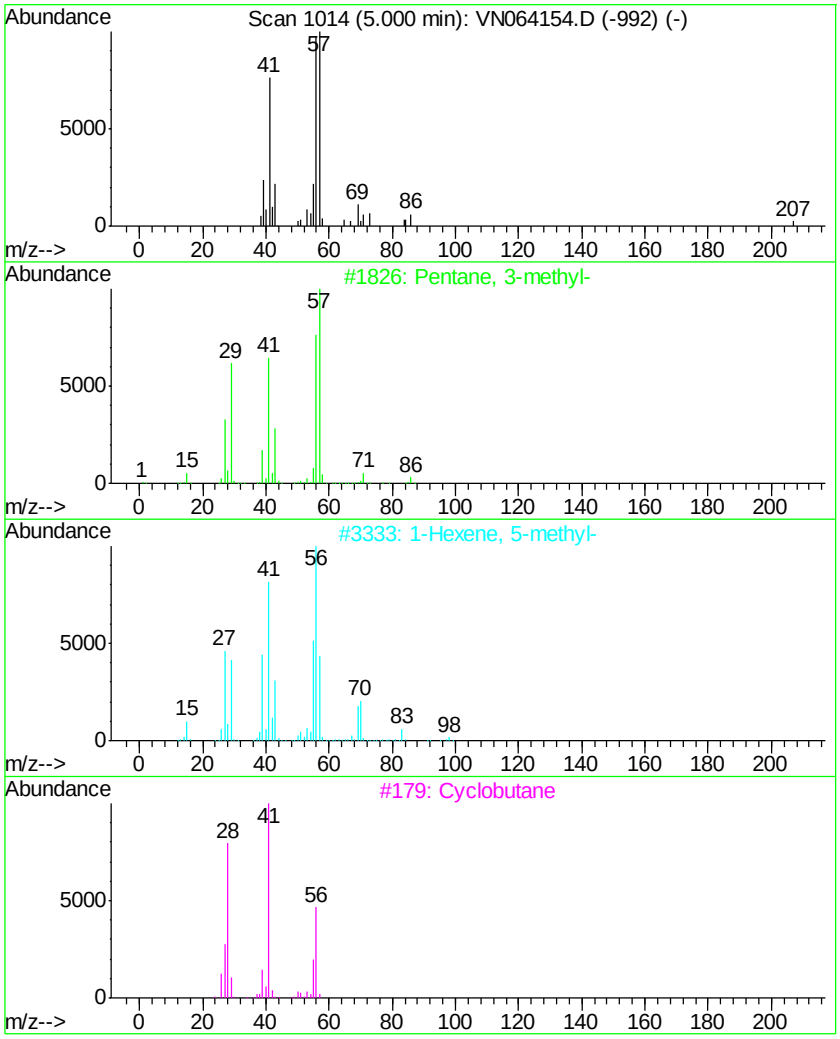
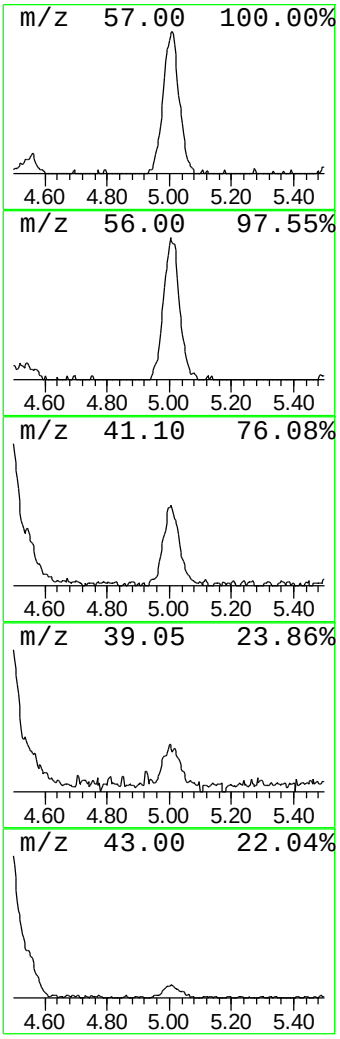
Peak Number 4 Pentane, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	6.39 ug/l	108689	Pentafluorobenzene	7.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	72
2	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	53
3	Cyclobutane	56	C4H8	000287-23-0	50
4	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	45
5	4-Penten-2-ol, 4-methyl-	100	C6H12O	002004-67-3	42





Library Search Compound Report

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Data File : VN064154.D
Acq On : 15 Oct 2020 19:31
Operator : JC/MD
Sample : L4417-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N101420W.M
Quant Title : SW846 8260

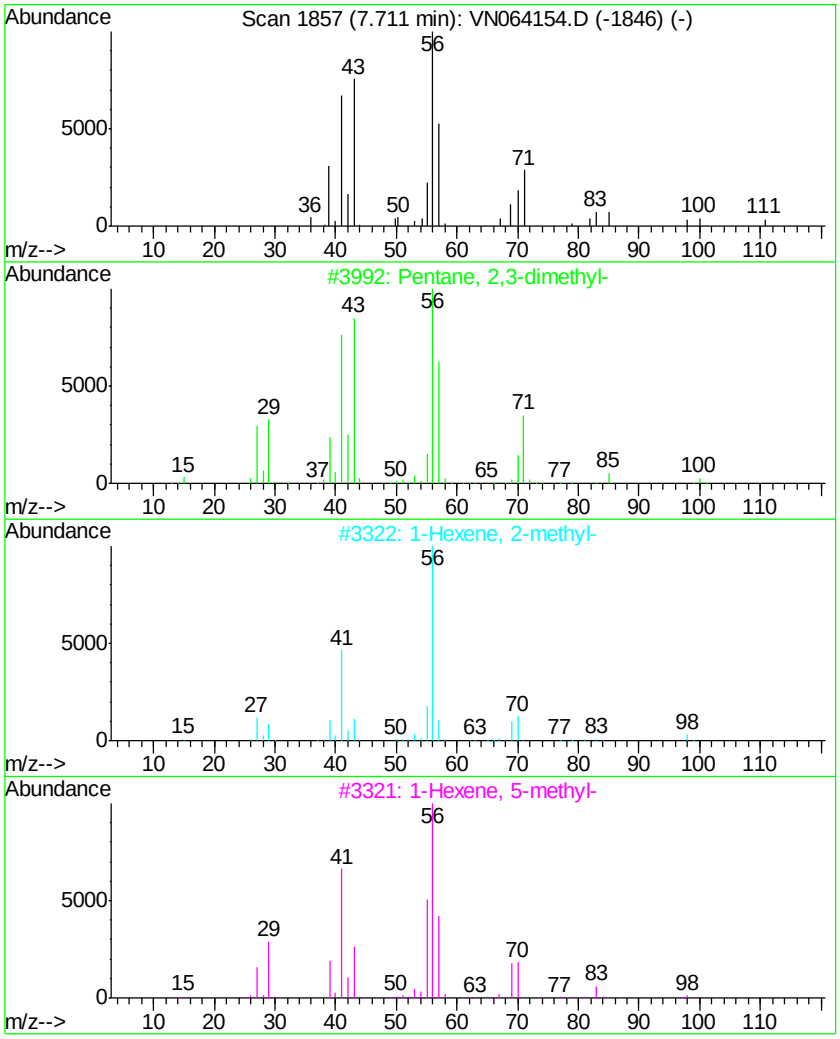
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

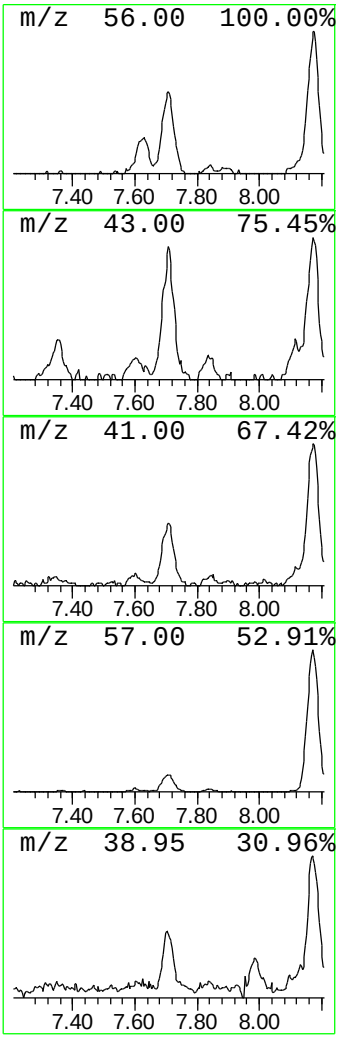
****

Peak Number 5 Pentane, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.71	5.33 ug/l	90586	Pentafluorobenzene	7.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	81
2	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	53
3	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	50
4	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	50
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	49





Library Search Compound Report

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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N101420W.M
Quant Title : SW846 8260

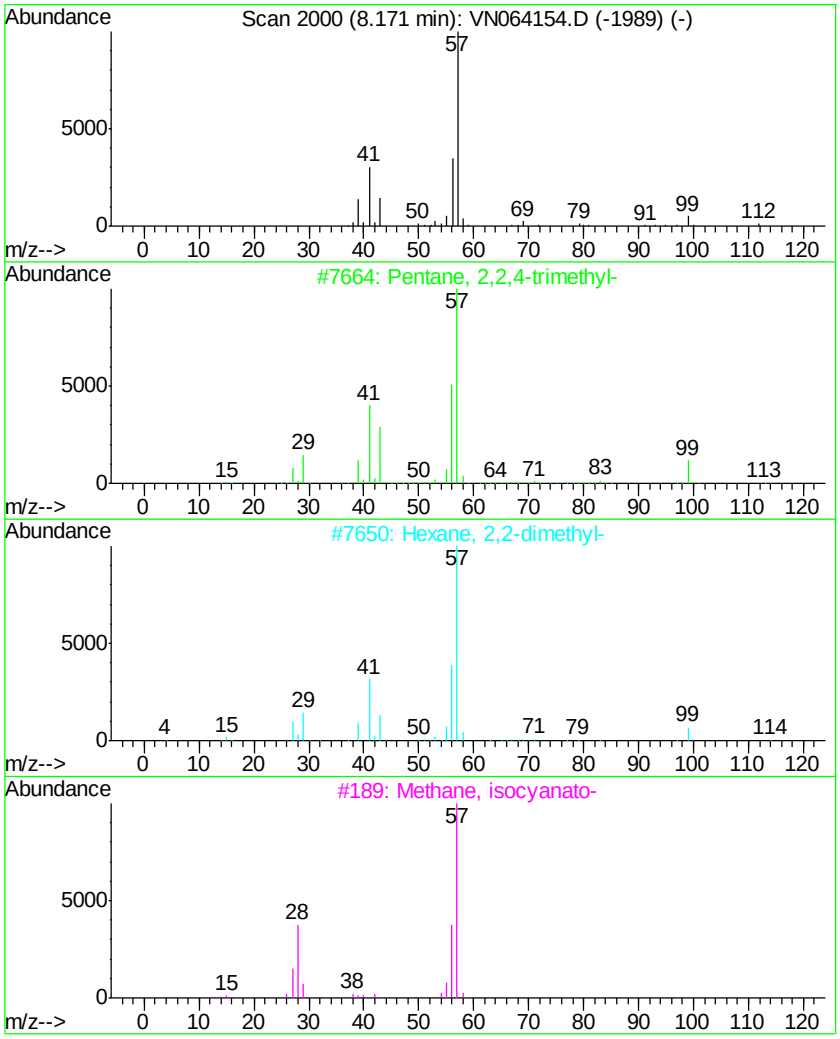
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

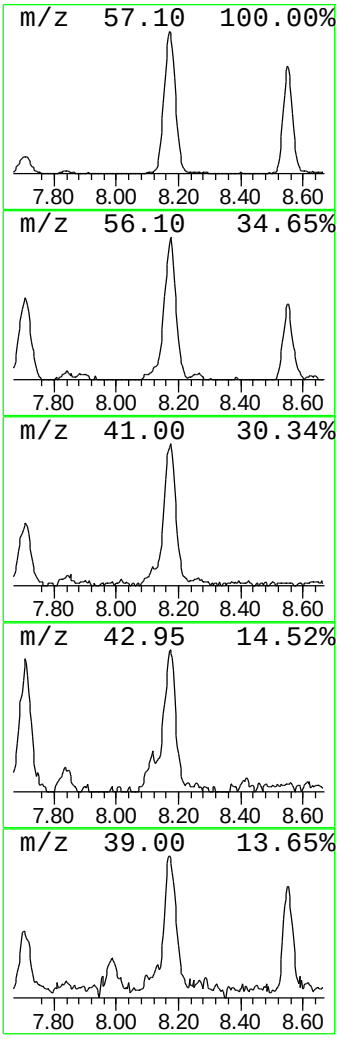
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.17	7.80 ug/l	196174	1,4-Difluorobenzene	8.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	64
2	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	64
3	Methane, isocyanato-	57	C2H3NO	000624-83-9	59
4	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	50
5	Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	45





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ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N101420W.M
Quant Title : SW846 8260

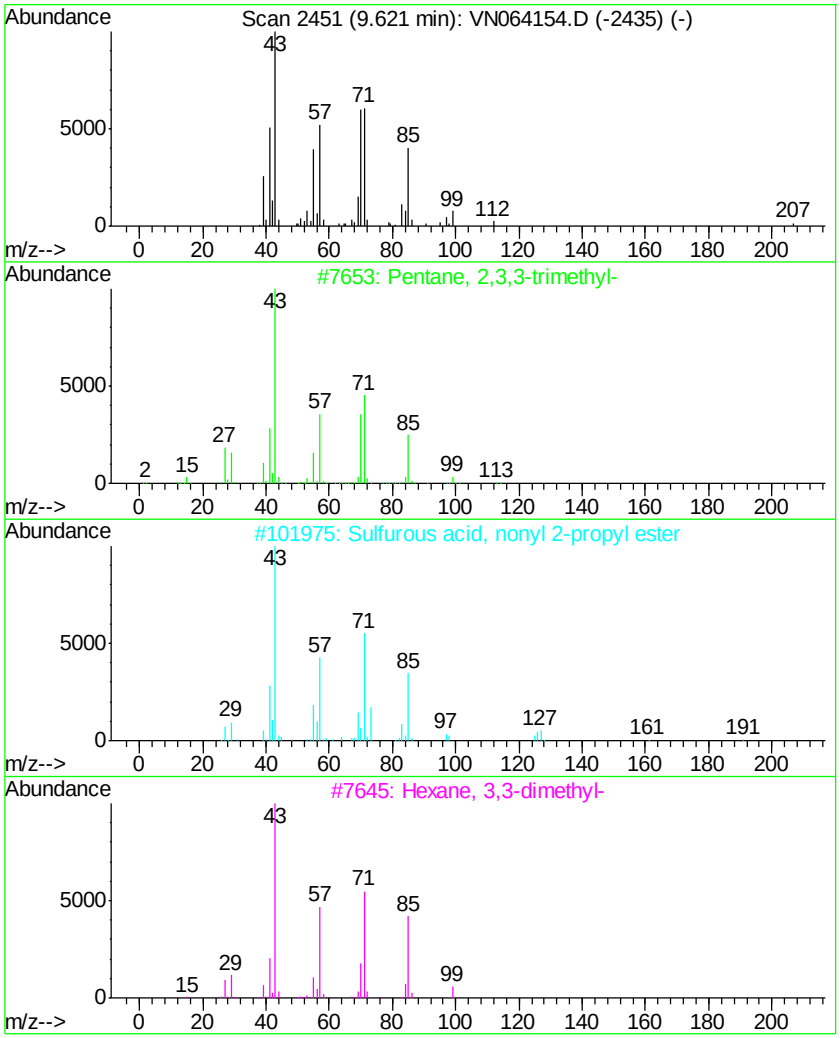
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

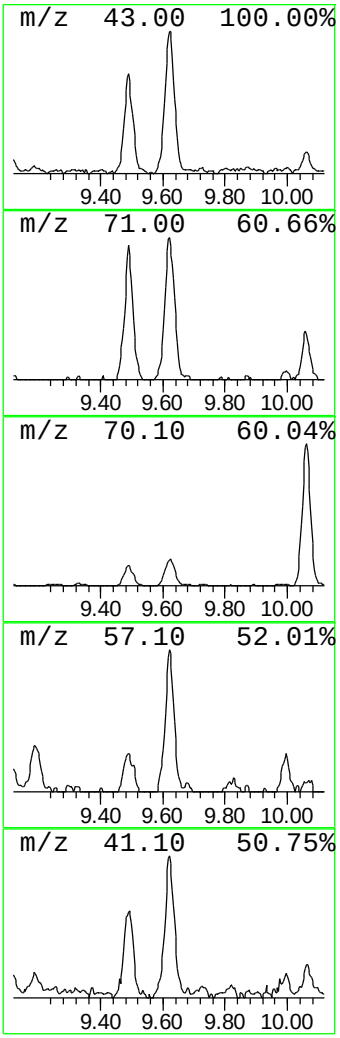
****

Peak Number 7 Pentane, 2,3,3-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.62	6.17 ug/l	155281	1,4-Difluorobenzene	8.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	72
2	Sulfurous acid, nonyl 2-propyl e...	250	C12H26O3S	1000309-12-0	53
3	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	50
4	Heptadecane, 7-methyl-	254	C18H38	020959-33-5	47
5	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	47





Tentatively Identified Compound (LSC) summary

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ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N101420W.M
Quant Title : SW846 8260

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methyl-	2.78	15.8	ug/l	269054	1	7.63	850303	50.0
Butane, 2,2-dimet...	3.77	15.3	ug/l	259401	1	7.63	850303	50.0
Butane, 2,3-dimet...	4.49	8.2	ug/l	138777	1	7.63	850303	50.0
Pentane, 3-methyl-	5.00	6.4	ug/l	108689	1	7.63	850303	50.0
Pentane, 2,3-dime...	7.71	5.3	ug/l	90586	1	7.63	850303	50.0
Pentane, 2,2,4-tr...	8.17	7.8	ug/l	196174	2	8.55	1258190	50.0
Pentane, 2,3,3-tr...	9.62	6.2	ug/l	155281	2	8.55	1258190	50.0