LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033121\
Data File : VN066440.D
Acq On : 31 Mar 2021 13:48
Operator : JC/MD
Sample : M1835-07 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : ASR8

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\82N032521W.M
Title : SW846 8260

Signal : TIC: VN066440.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	153	168	184	rVB	259964	380096	4.95%	1.000%
2	2.754	381	397	420	rVB	543331	1077224	14.03%	2.834%
3	3.004	478	490	503	rBV3	40357	78464	1.02%	0.206%
4	3.081	504	519	547	rVB3	175068	396913	5.17%	1.044%
5	3.256	567	584	605	rBV	230757	493544	6.43%	1.298%
6	3.409	627	641	656	rVV2	110206	237246	3.09%	0.624%
7	3.494	657	673	693	rVB2	165732	390029	5.08%	1.026%
8	4.331	968	985	1003	rVB4	90568	239859	3.12%	0.631%
9	4.940	1181	1212	1246	rBV2	112695	412791	5.37%	1.086%
10	6.522	1778	1802	1828	rVB4	76023	246788	3.21%	0.649%
11	7.507	2144	2169	2182	rBV	315612	798492	10.40%	2.100%
12	7.582	2183	2197	2218	rVV	552128	1366668	17.79%	3.595%
13	7.960	2311	2338	2364	rBV3	1857941	4610140	60.02%	12.127%
14	8.075	2367	2381	2391	rBV7	37643	99830	1.30%	0.263%
15	8.512	2519	2544	2569	rBV	764512	1584534	20.63%	4.168%
16	9.011	2701	2730	2744	rBV5	38695	107234	1.40%	0.282%
17	9.588	2918	2945	2963	rVV4	61122	153350	2.00%	0.403%
18	10.028	3092	3109	3121	rBV	1318462	2390486	31.12%	6.288%
19	10.092	3121	3133	3152	rVB	1489121	2663982	34.68%	7.008%
20	11.347	3584	3601	3624	rBV	981727	1720209	22.40%	4.525%
21	11.452	3625	3640	3661	rVV	1226605	2030422	26.44%	5.341%
22	11.559	3663	3680	3709	rBV	4173837	7680641	100.00%	20.204%
23	11.889	3788	3803	3831	rBV	1016141	1684961	21.94%	4.432%
24	12.192	3901	3916	3931	rBV2	49646	87086	1.13%	0.229%
25	12.345	3955	3973	3995	rBV2	799226	1394810	18.16%	3.669%
26	12.538	4031	4045	4055	rBV	109799	181980	2.37%	0.479%
27	12.600	4056	4068	4076	rBV	436380	733690	9.55%	1.930%
28	12.678	4088	4097	4122	rVB	302926	513459	6.69%	1.351%
29	12.836	4142	4156	4172	rBV	191156	333009	4.34%	0.876%
30	12.983	4196	4211	4242	rBV	957693	1586545	20.66%	4.173%
31	13.286	4310	4324	4333	rBV	743022	1377191	17.93%	3.623%
32	13.487	4380	4399	4409	rBV	277808	510396	6.65%	1.343%
33	13.833	4519	4528	4543	rBV	59486	98167	1.28%	0.258%
34	14.193	4655	4662	4675	rVB	51662	79196	1.03%	0.208%
35	14.536	4778	4790	4808	rBV4	69356	137386	1.79%	0.361%
36	15.073	4982	4990	5009	rVB	73118	139223	1.81%	0.366%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033121\
Data File : VN066440.D
Acq On : 31 Mar 2021 13:48
Operator : JC/MD
Sample : M1835-07 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ASR8

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\82N032521W.M
Title : SW846 8260

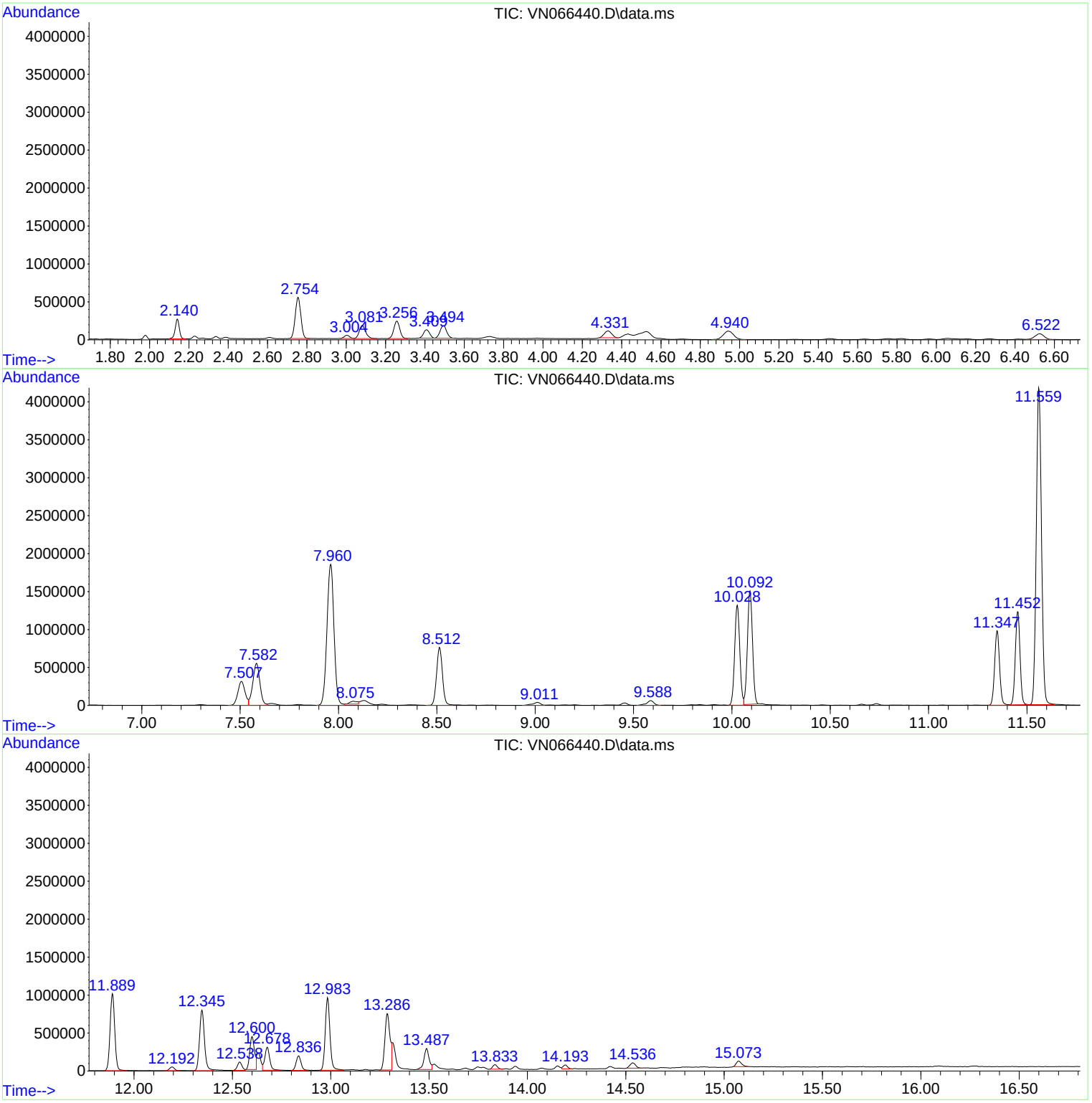
Sum of corrected areas: 38016041

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033121\
Data File : VN066440.D
Acq On : 31 Mar 2021 13:48
Operator : JC/MD
Sample : M1835-07 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ASR8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033121\
Data File : VN066440.D
Acq On : 31 Mar 2021 13:48
Operator : JC/MD
Sample : M1835-07 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ASR8

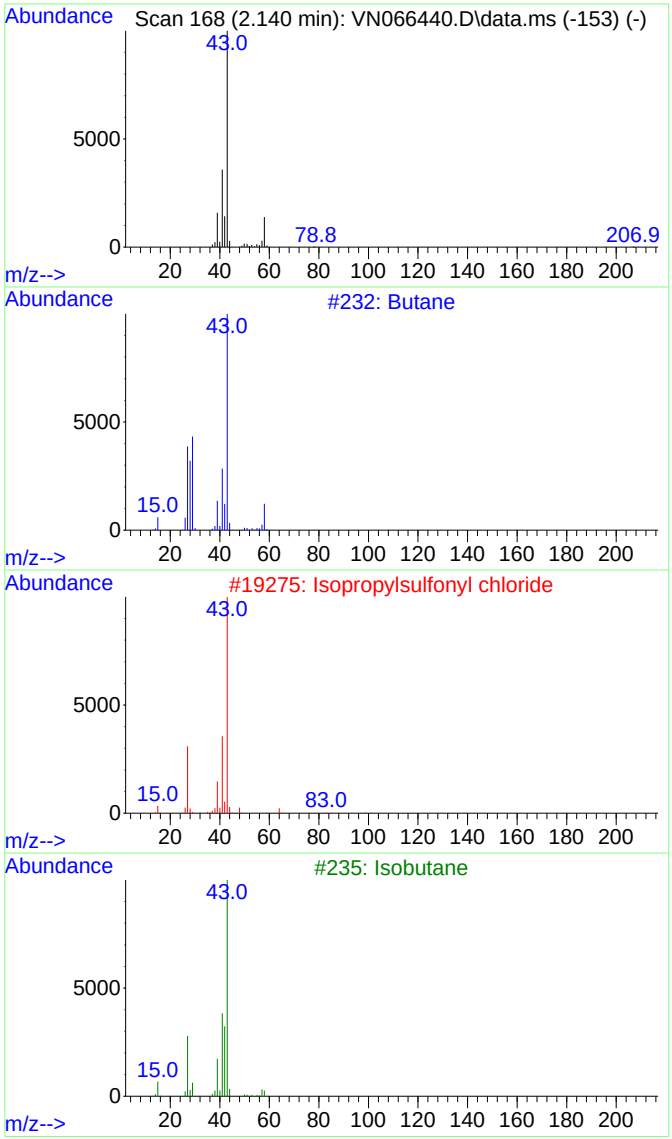
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

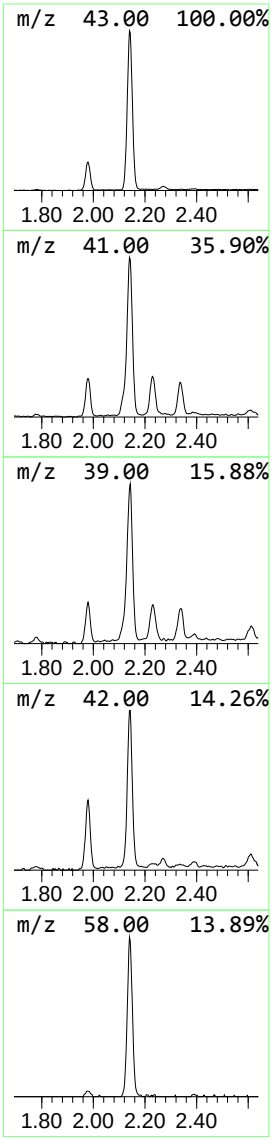
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	13.91 ug/l	380096	Pentafluorobenzene	7.584

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	72
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	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033121\
Data File : VN066440.D
Acq On : 31 Mar 2021 13:48
Operator : JC/MD
Sample : M1835-07 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : ASR8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

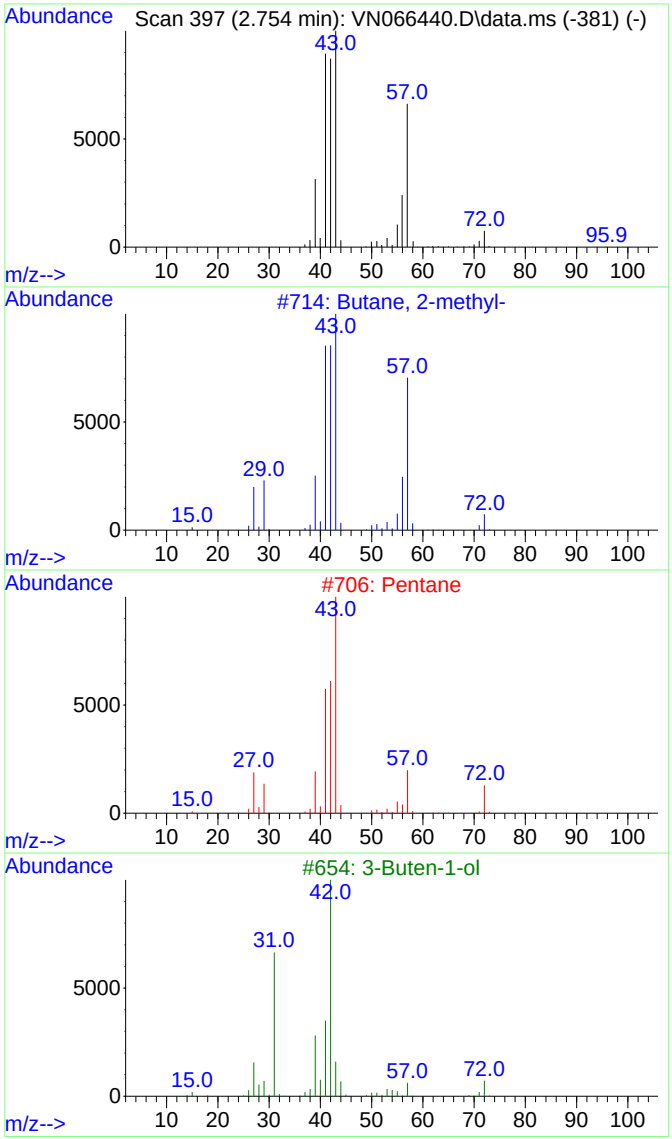
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

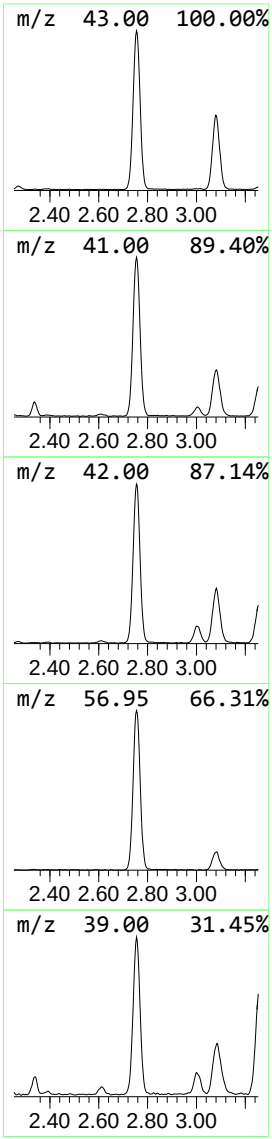
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.754	39.41 ug/l	1077220	Pentafluorobenzene	7.584

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	94
2	Pentane	72	C5H12	000109-66-0	64
3	3-Buten-1-ol	72	C4H8O	000627-27-0	47
4	Propane, 2-methyl-1-nitro-	103	C4H9NO2	000625-74-1	10
5	1-Butene	56	C4H8	000106-98-9	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033121\
Data File : VN066440.D
Acq On : 31 Mar 2021 13:48
Operator : JC/MD
Sample : M1835-07 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : ASR8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

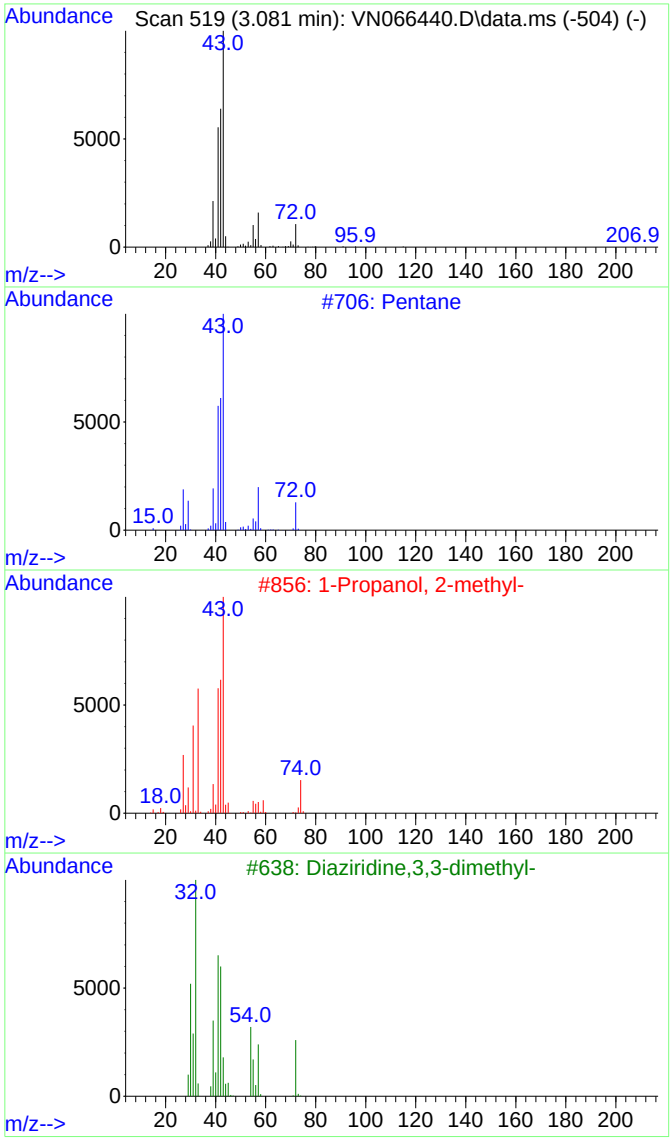
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

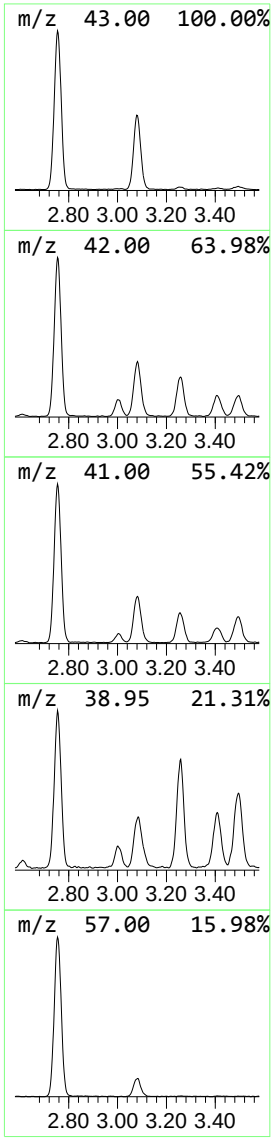
****

Peak Number 3 Pentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.081	14.52 ug/l	396913	Pentafluorobenzene	7.584

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	90
2	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	39
3	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
4	1-Pentene, 4-methyl-	84	C6H12	000691-37-2	23
5	Butanal, 2,2-dimethyl-	100	C6H12O	002094-75-9	12





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033121\
Data File : VN066440.D
Acq On : 31 Mar 2021 13:48
Operator : JC/MD
Sample : M1835-07 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : ASR8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

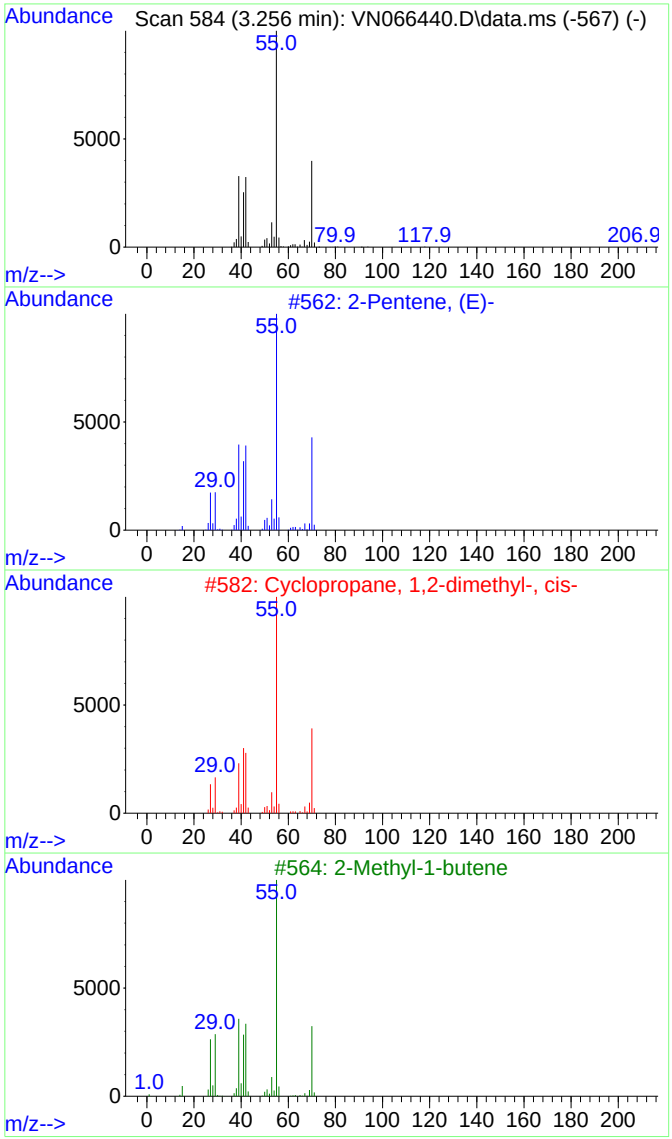
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

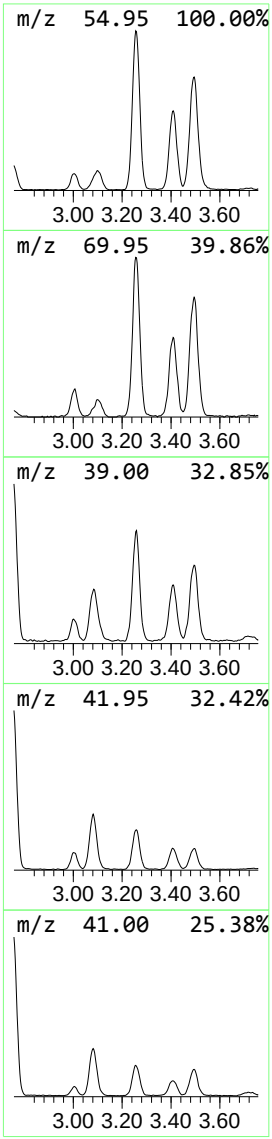
****

Peak Number 4 2-Pentene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.256	18.06 ug/l	493544	Pentafluorobenzene	7.584

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, (E)-	70	C5H10	000646-04-8	93
2	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	90
3	2-Methyl-1-butene	70	C5H10	000563-46-2	87
4	2-Butene, 2-methyl-	70	C5H10	000513-35-9	87
5	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	81





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033121\
Data File : VN066440.D
Acq On : 31 Mar 2021 13:48
Operator : JC/MD
Sample : M1835-07 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : ASR8

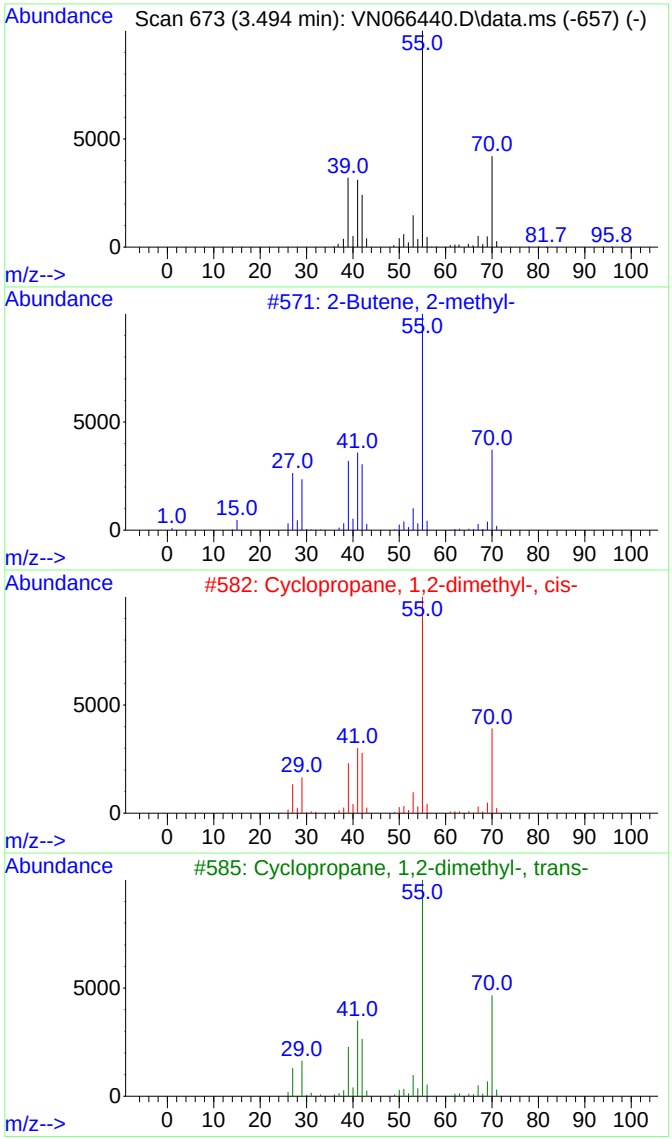
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

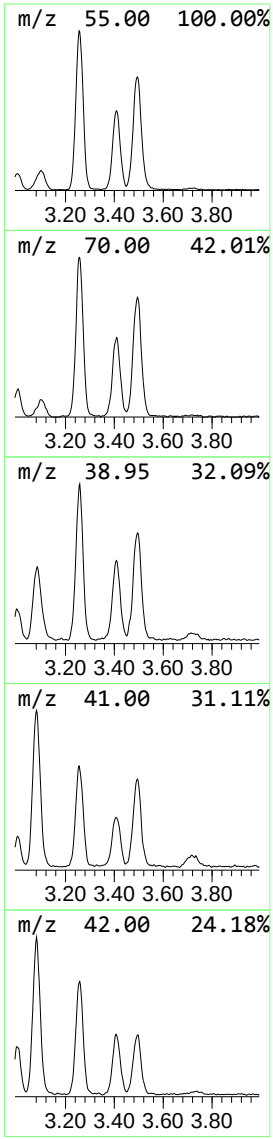
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Butene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.494	14.27 ug/l	390029	Pentafluorobenzene	7.584

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene, 2-methyl-	70	C5H10	000513-35-9	91
2	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
3	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	91
4	2-Pentene, (E)-	70	C5H10	000646-04-8	86
5	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033121\
Data File : VN066440.D
Acq On : 31 Mar 2021 13:48
Operator : JC/MD
Sample : M1835-07 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : ASR8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

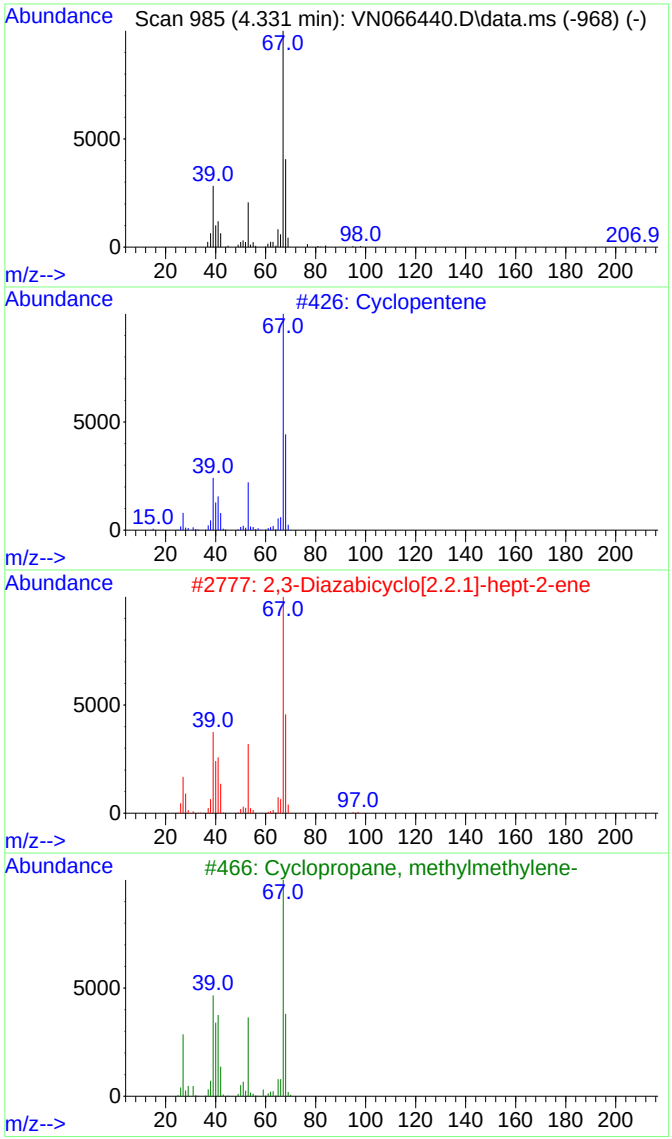
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

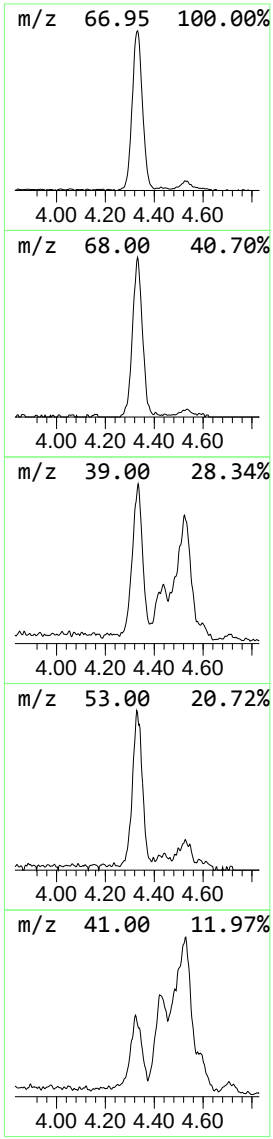
****

Peak Number 6 Cyclopentene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.331	8.78 ug/l	239859	Pentafluorobenzene	7.584

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene	68	C5H8	000142-29-0	91
2	2,3-Diazabicyclo[2.2.1]-hept-2-ene	96	C5H8N2	002721-32-6	83
3	Cyclopropane, methylmethylene-	68	C5H8	018631-84-0	64
4	1,4-Pentadiene	68	C5H8	000591-93-5	58
5	1,3-Pentadiene	68	C5H8	000504-60-9	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033121\
Data File : VN066440.D
Acq On : 31 Mar 2021 13:48
Operator : JC/MD
Sample : M1835-07 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : ASR8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

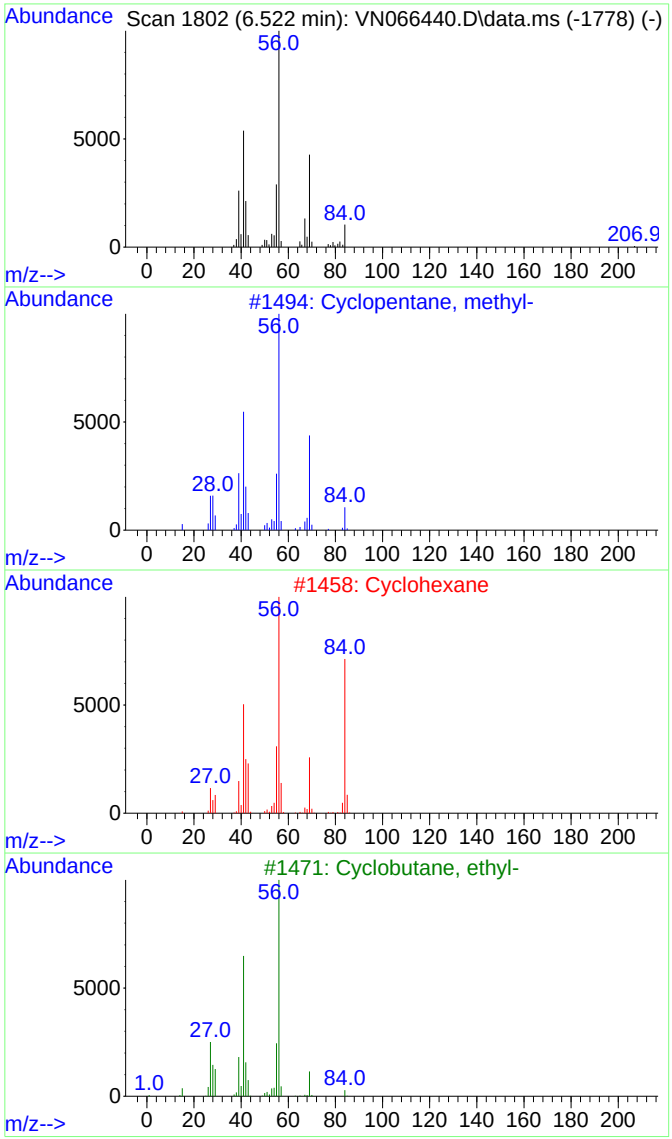
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

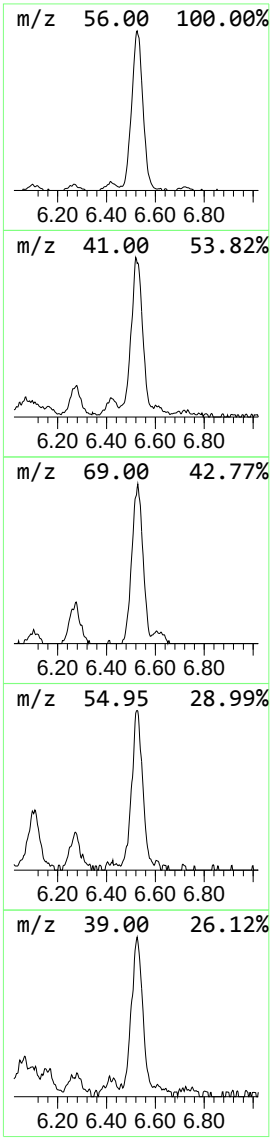
****

Peak Number 7 Cyclopentane, methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.522	9.03 ug/l	246788	Pentafluorobenzene	7.584

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2	Cyclohexane	84	C6H12	000110-82-7	78
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	59
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033121\
Data File : VN066440.D
Acq On : 31 Mar 2021 13:48
Operator : JC/MD
Sample : M1835-07 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ASR8

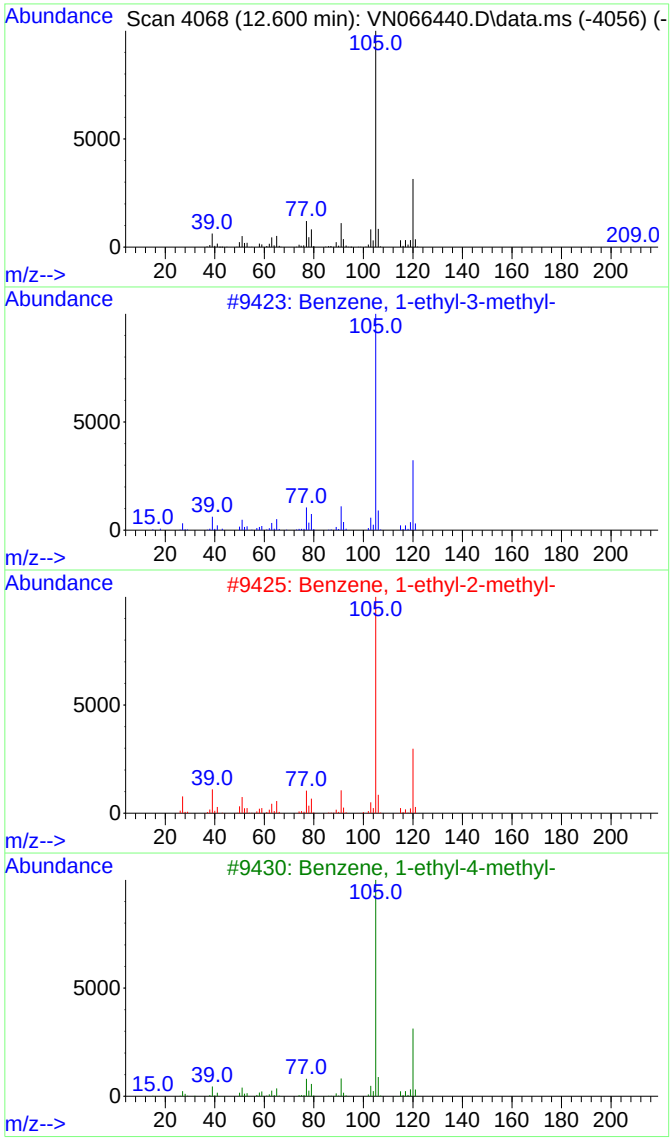
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

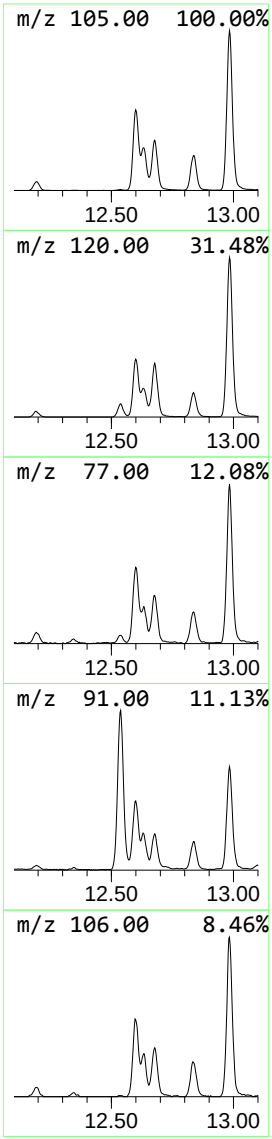
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1-ethyl-3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.600	26.64 ug/l	733690	1,4-Dichlorobenzene-d4	13.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	97
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033121\
Data File : VN066440.D
Acq On : 31 Mar 2021 13:48
Operator : JC/MD
Sample : M1835-07 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : ASR8

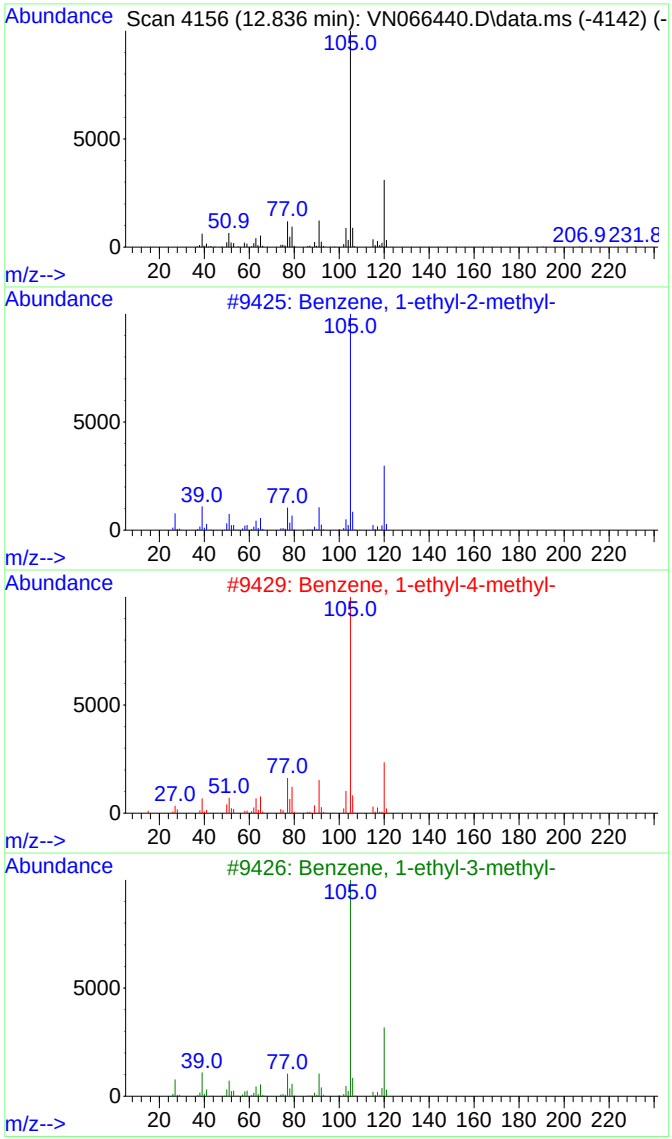
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

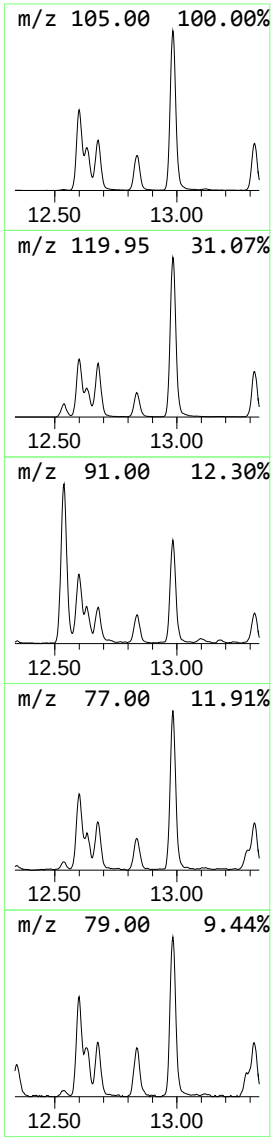
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.836	12.09 ug/l	333009	1,4-Dichlorobenzene-d4	13.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033121\
Data File : VN066440.D
Acq On : 31 Mar 2021 13:48
Operator : JC/MD
Sample : M1835-07 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : ASR8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

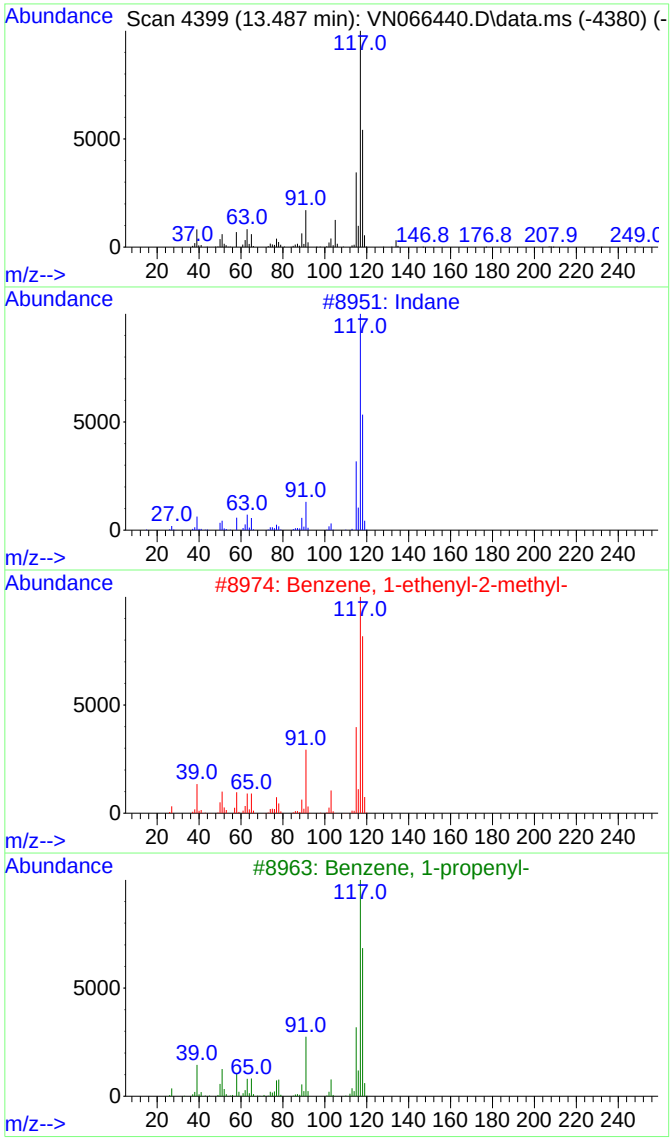
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

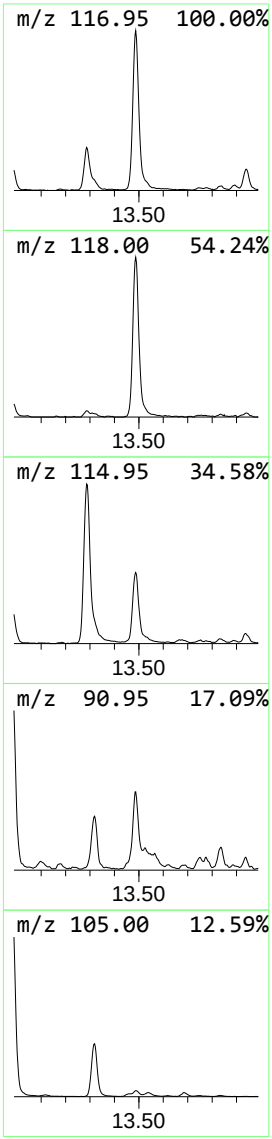
****

Peak Number 10 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.488	18.53 ug/l	510396	1,4-Dichlorobenzene-d4	13.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	95
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	78
3	Benzene, 1-propenyl-	118	C9H10	000637-50-3	74
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
5	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033121\
Data File : VN066440.D
Acq On : 31 Mar 2021 13:48
Operator : JC/MD
Sample : M1835-07 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : ASR8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.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	2.140	13.9	ug/l	380096	1	7.584	1366670	50.0
Butane, 2-methyl-	2.754	39.4	ug/l	1077220	1	7.584	1366670	50.0
Pentane	3.081	14.5	ug/l	396913	1	7.584	1366670	50.0
2-Pentene, (E)-	3.256	18.1	ug/l	493544	1	7.584	1366670	50.0
2-Butene, 2-met...	3.494	14.3	ug/l	390029	1	7.584	1366670	50.0
Cyclopentene	4.331	8.8	ug/l	239859	1	7.584	1366670	50.0
Cyclopentane, m...	6.522	9.0	ug/l	246788	1	7.584	1366670	50.0
Benzene, 1-ethy...	12.600	26.6	ug/l	733690	4	13.286	1377190	50.0
Benzene, 1-ethy...	12.836	12.1	ug/l	333009	4	13.286	1377190	50.0
Indane	13.488	18.5	ug/l	510396	4	13.286	1377190	50.0