LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032921\
Data File : VN066381.D
Acq On : 29 Mar 2021 16:58
Operator : JC/MD
Sample : M1835-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : ASR4

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: VN066381.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.752	378	396	417	rBV	1572159	3115972	1.62%	0.372%
2	3.087	502	521	549	rVB4	868012	2512184	1.31%	0.300%
3	3.256	567	584	607	rVB	1008331	2095640	1.09%	0.250%
4	3.492	654	672	702	rVB	2732235	6362274	3.31%	0.760%
5	4.329	958	984	1004	rBV	946804	2783737	1.45%	0.333%
6	4.943	1177	1213	1247	rBV3	632260	2284456	1.19%	0.273%
7	6.525	1780	1803	1824	rBV2	1185983	3612947	1.88%	0.432%
8	7.300	2074	2092	2115	rVB2	773659	2002433	1.04%	0.239%
9	7.571	2178	2193	2213	rVB7	1200014	3472681	1.81%	0.415%
10	7.963	2313	2339	2366	rBV	23754342	59951351	31.22%	7.166%
11	8.129	2367	2401	2425	rVB4	1220766	5843363	3.04%	0.698%
12	8.510	2523	2543	2571	rBV3	1401661	3667382	1.91%	0.438%
13	9.011	2697	2730	2744	rBV4	1088656	3102220	1.62%	0.371%
14	9.454	2882	2895	2915	rVB	988059	1949515	1.02%	0.233%
15	9.588	2937	2945	2964	rVB2	1393733	3013701	1.57%	0.360%
16	10.028	3095	3109	3118	rBV2	1643063	3018546	1.57%	0.361%
17	10.095	3118	3134	3165	rVB	37439502	74427966	38.76%	8.896%
18	10.736	3355	3373	3395	rBV	4533929	8104862	4.22%	0.969%
19	11.350	3587	3602	3623	rBV	1238474	2410442	1.26%	0.288%
20	11.455	3624	3641	3663	rBV	38721110	67721027	35.26%	8.094%
21	11.567	3664	3683	3711	rVV2	83193056	192035944	100.00%	22.953%
22	11.892	3786	3804	3830	rBV	41726209	73642880	38.35%	8.802%
23	12.192	3903	3916	3929	rBV	2531924	4061005	2.11%	0.485%
24	12.535	4030	4044	4055	rBV	5589662	8805868	4.59%	1.053%
25	12.600	4055	4068	4075	rBV	20931954	34548154	17.99%	4.129%
26	12.678	4088	4097	4114	rVB	17093469	27150245	14.14%	3.245%
27	12.836	4141	4156	4177	rBV	11203226	18586486	9.68%	2.222%
28	12.986	4196	4212	4242	rVB	44252449	73641809	38.35%	8.802%
29	13.316	4313	4335	4357	rBV	16230418	28577995	14.88%	3.416%
30	13.485	4375	4398	4407	rBV	13875179	25656349	13.36%	3.067%
31	13.528	4408	4414	4436	rVB2	5625596	9748093	5.08%	1.165%
32	13.681	4456	4471	4483	rVB2	1762512	3420564	1.78%	0.409%
33	13.745	4483	4495	4501	rBV	3269149	5109669	2.66%	0.611%
34	13.831	4516	4527	4539	rVB	5750853	8617043	4.49%	1.030%
35	13.938	4556	4567	4581	rVB2	3480490	5628878	2.93%	0.673%
36	14.070	4604	4616	4629	rBV	1587597	2490097	1.30%	0.298%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032921\
Data File : VN066381.D
Acq On : 29 Mar 2021 16:58
Operator : JC/MD
Sample : M1835-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : ASR4

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

37	14.153	4634	4647	4653	rBV	3454162	5205946	2.71%	0.622%
38	14.190	4654	4661	4672	rVB	4504152	6555248	3.41%	0.784%
39	14.418	4735	4746	4757	rBV	3032039	4640625	2.42%	0.555%
40	14.534	4773	4789	4803	rBV3	6044934	11633067	6.06%	1.390%
41	14.794	4865	4886	4893	rBV5	1017339	2280786	1.19%	0.273%
42	15.067	4974	4988	5006	rBV	8113676	14376683	7.49%	1.718%
43	16.078	5350	5365	5401	rVB	2850164	5776284	3.01%	0.690%
44	16.266	5420	5435	5460	rVB	1417555	3004393	1.56%	0.359%

Sum of corrected areas: 836646810

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Data File : VN066381.D
Acq On : 29 Mar 2021 16:58
Operator : JC/MD
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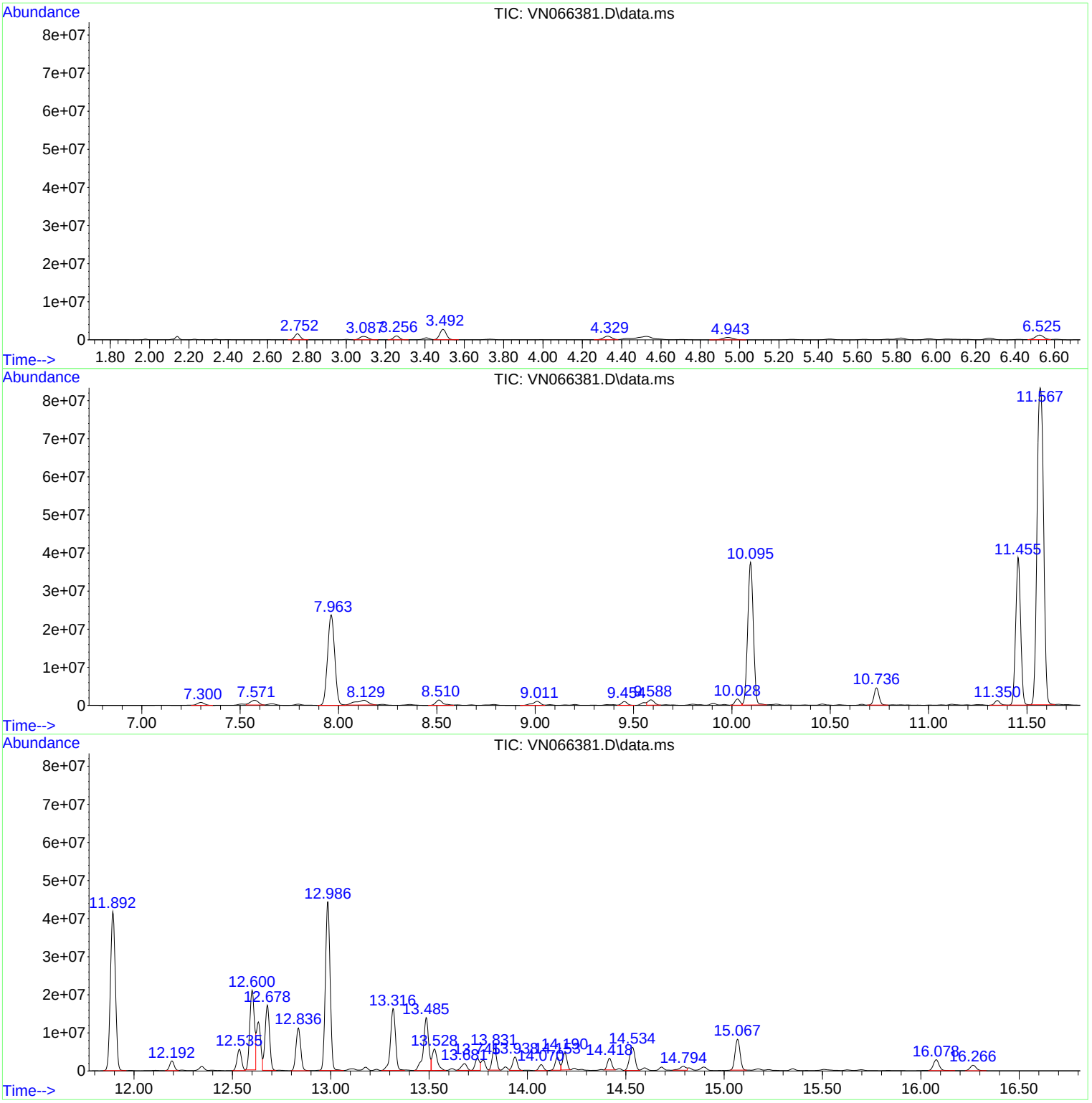
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ASR4

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\VN032921\
Data File : VN066381.D
Acq On : 29 Mar 2021 16:58
Operator : JC/MD
Sample : M1835-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ASR4

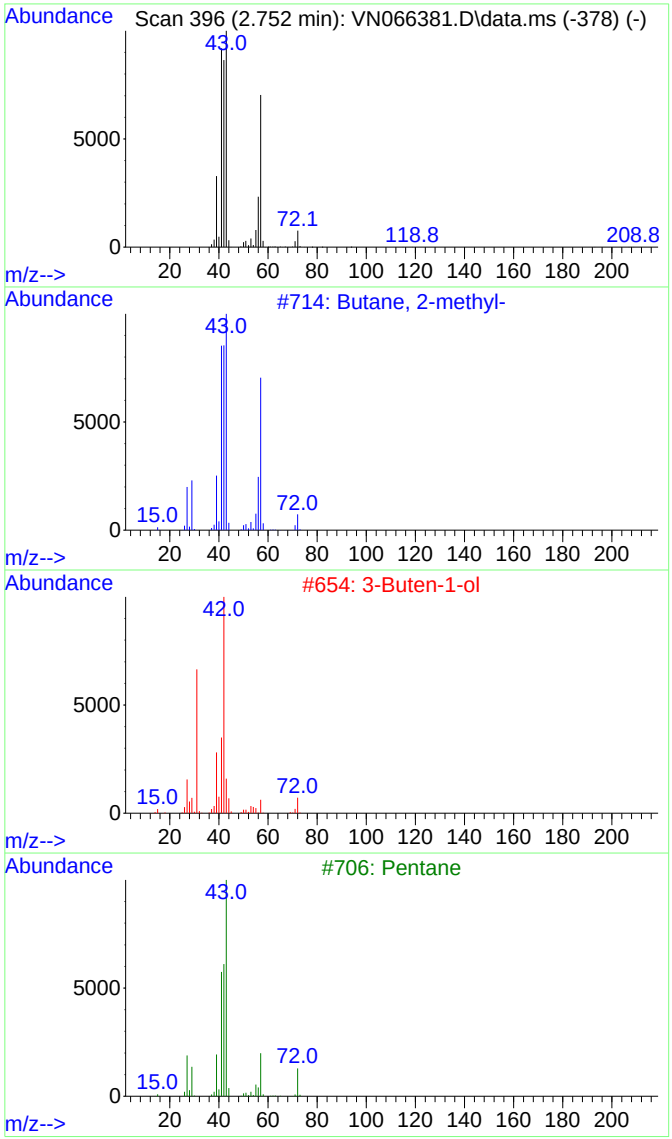
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

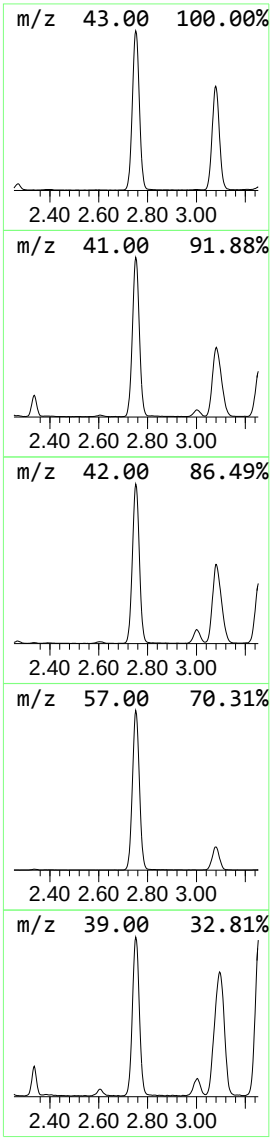
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.752	44.86 ug/l	3115970	Pentafluorobenzene	7.585

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	36
4	1-Butene	56	C4H8	000106-98-9	9
5	Methane, isocyanato-	57	C2H3NO	000624-83-9	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032921\
Data File : VN066381.D
Acq On : 29 Mar 2021 16:58
Operator : JC/MD
Sample : M1835-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ASR4

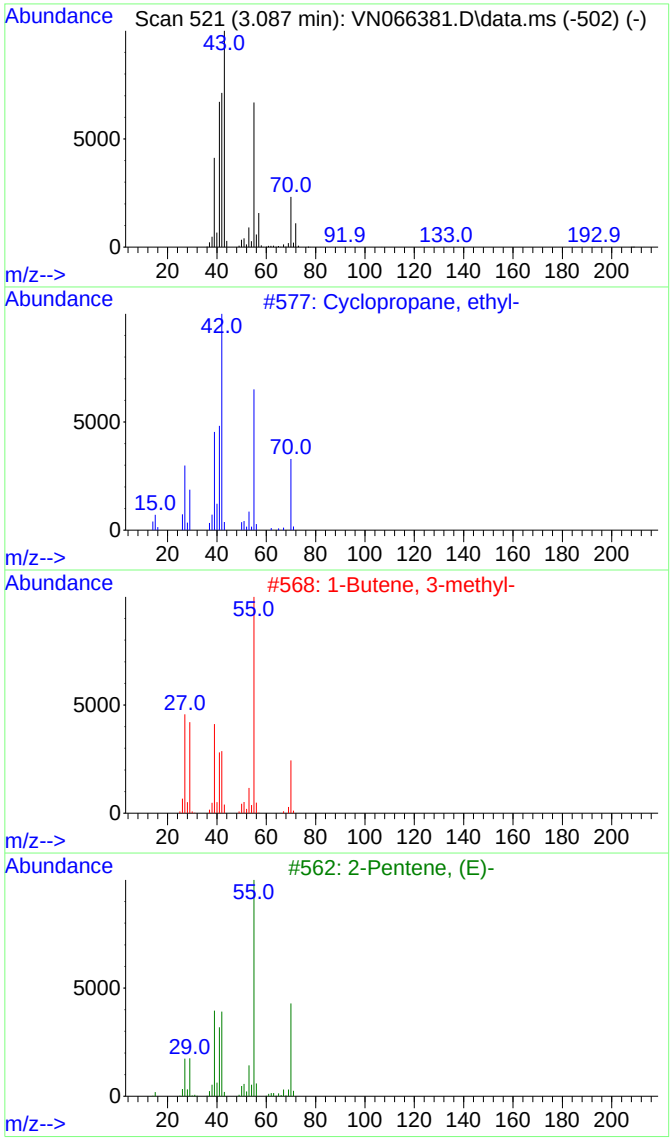
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

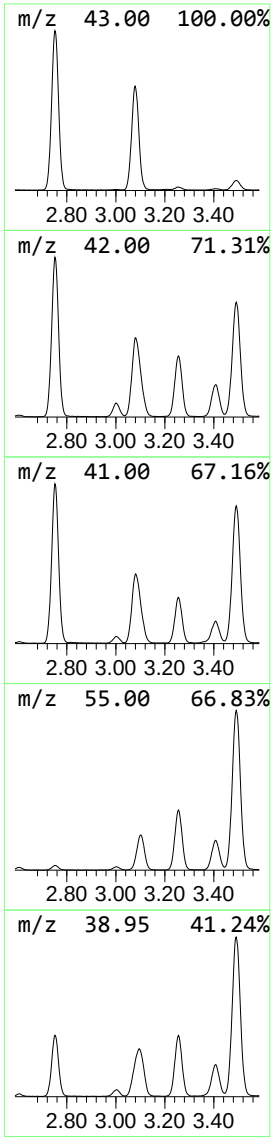
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclopropane, ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.087	36.17 ug/l	2512180	Pentafluorobenzene	7.585

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, ethyl-	70	C5H10	001191-96-4	58
2	1-Butene, 3-methyl-	70	C5H10	000563-45-1	52
3	2-Pentene, (E)-	70	C5H10	000646-04-8	46
4	Cyclobutane, methyl-	70	C5H10	000598-61-8	43
5	Pentane	72	C5H12	000109-66-0	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032921\
Data File : VN066381.D
Acq On : 29 Mar 2021 16:58
Operator : JC/MD
Sample : M1835-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ASR4

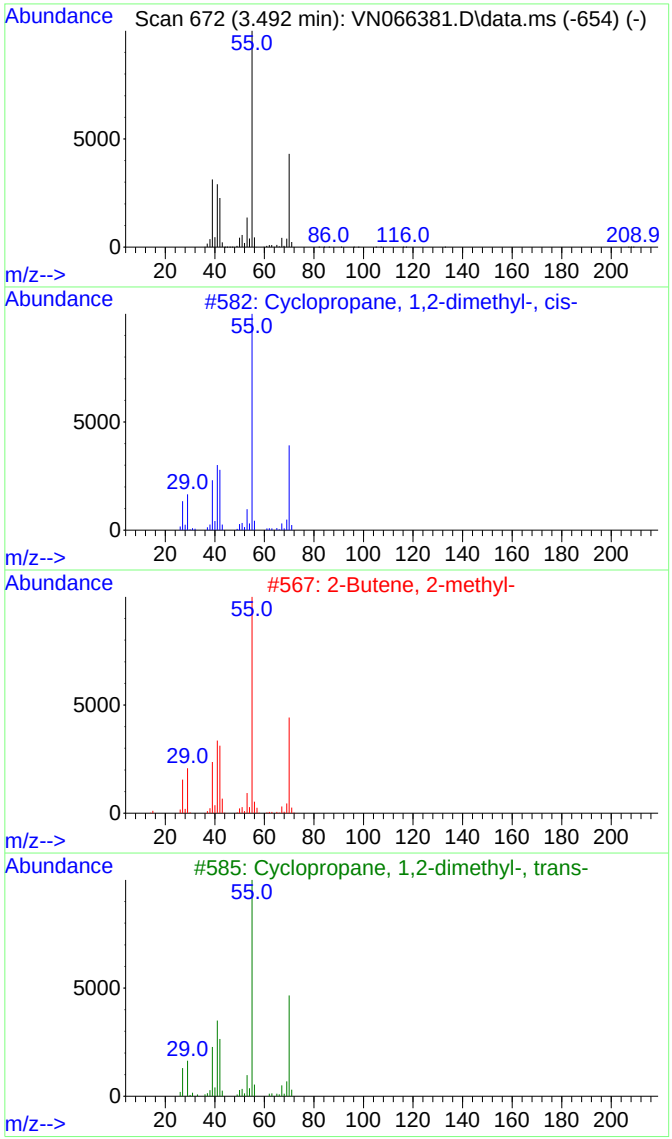
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

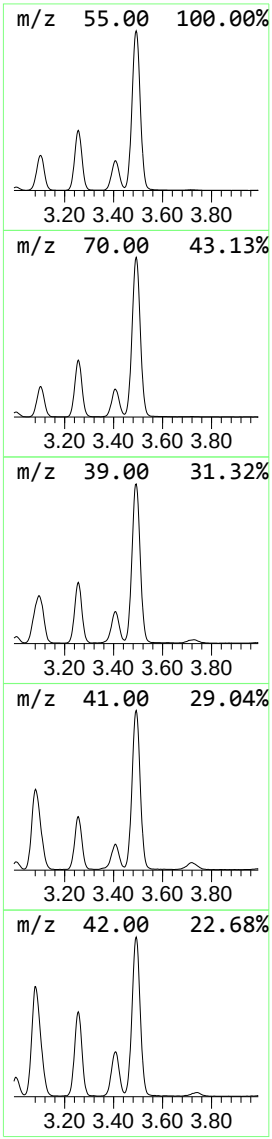
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopropane, 1,2-dimethyl-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.492	91.60 ug/l	6362270	Pentafluorobenzene	7.585

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
2	2-Butene, 2-methyl-	70	C5H10	000513-35-9	87
3	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	83
4	1-Butene, 3-methyl-	70	C5H10	000563-45-1	78
5	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032921\
Data File : VN066381.D
Acq On : 29 Mar 2021 16:58
Operator : JC/MD
Sample : M1835-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : ASR4

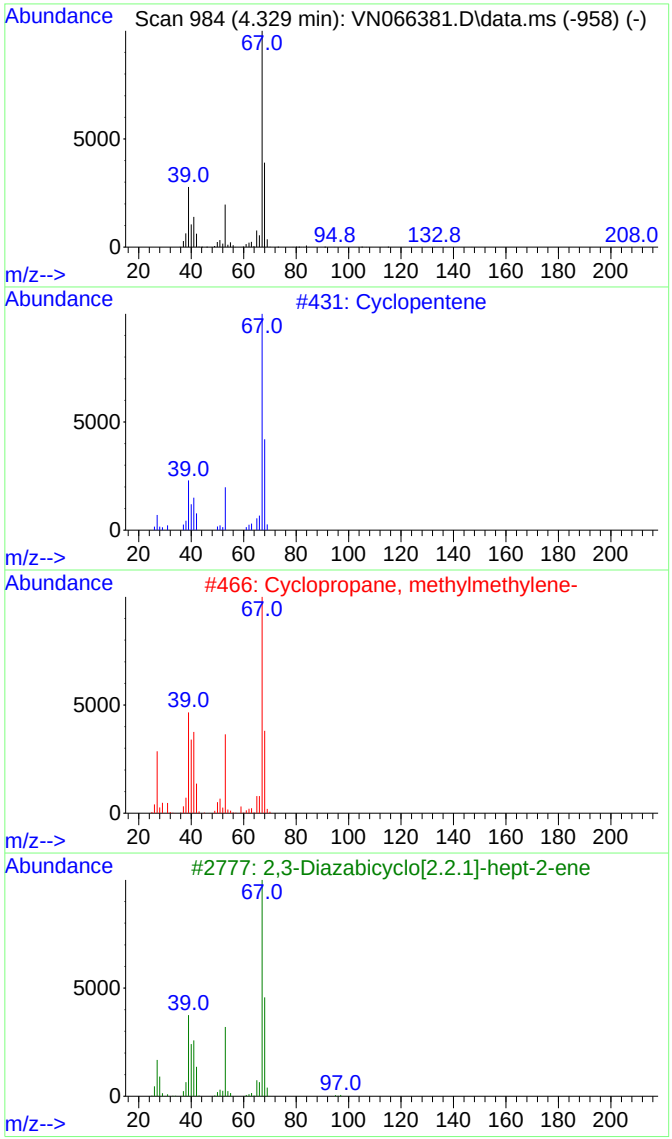
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

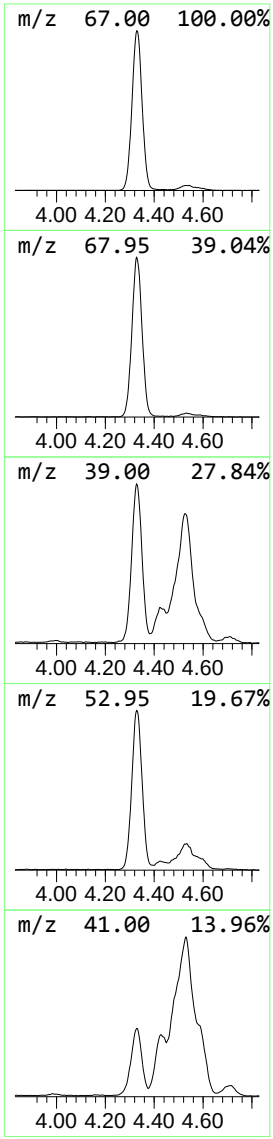
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopentene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.329	40.08 ug/l	2783740	Pentafluorobenzene	7.585

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene	68	C5H8	000142-29-0	91
2	Cyclopropane, methylmethylene-	68	C5H8	018631-84-0	91
3	2,3-Diazabicyclo[2.2.1]-hept-2-ene	96	C5H8N2	002721-32-6	83
4	1,4-Pentadiene	68	C5H8	000591-93-5	64
5	1-Butyne, 3-methyl-	68	C5H8	000598-23-2	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032921\
Data File : VN066381.D
Acq On : 29 Mar 2021 16:58
Operator : JC/MD
Sample : M1835-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ASR4

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

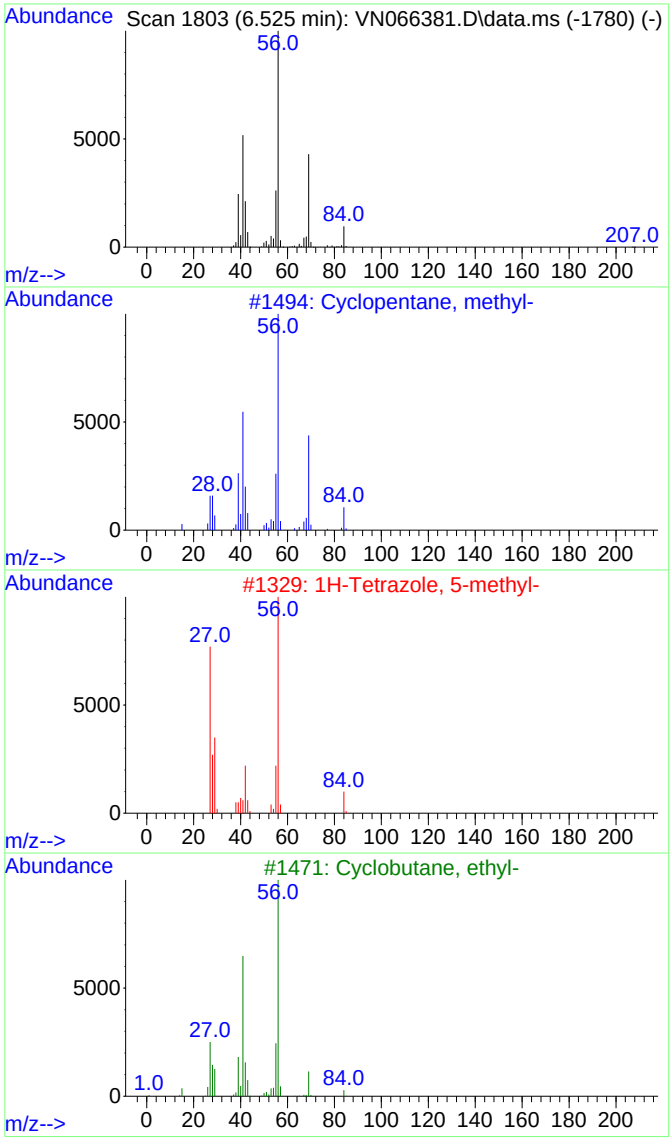
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

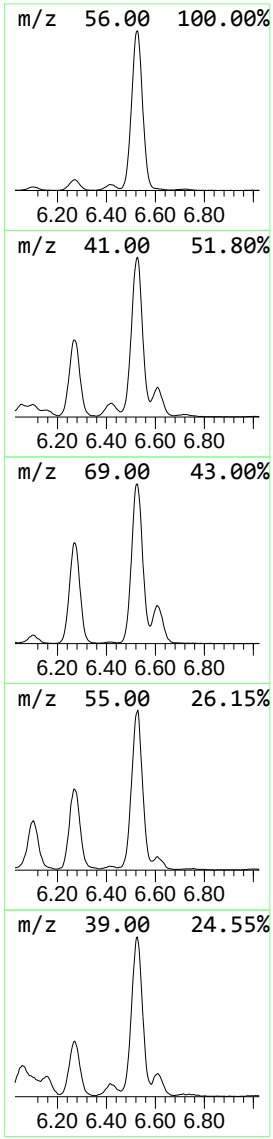
****

Peak Number 5 Cyclopentane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.525	52.02 ug/l	3612950	Pentafluorobenzene	7.585

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
4	Cyclohexane	84	C6H12	000110-82-7	56
5	Cyclopropane, propyl-	84	C6H12	002415-72-7	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032921\
Data File : VN066381.D
Acq On : 29 Mar 2021 16:58
Operator : JC/MD
Sample : M1835-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ASR4

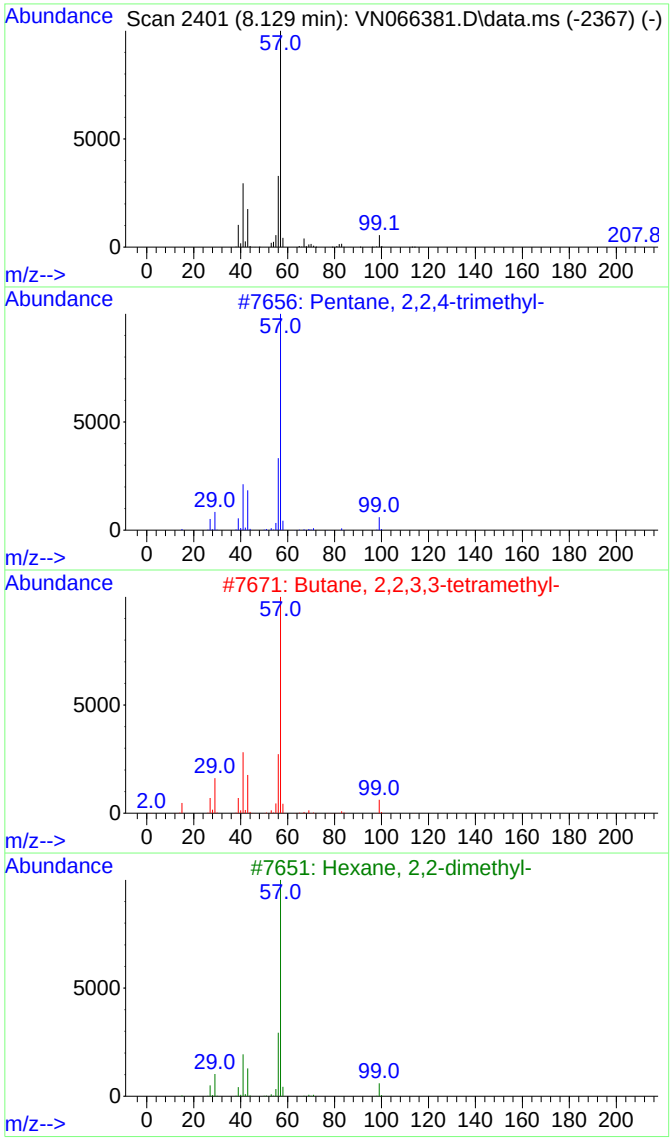
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

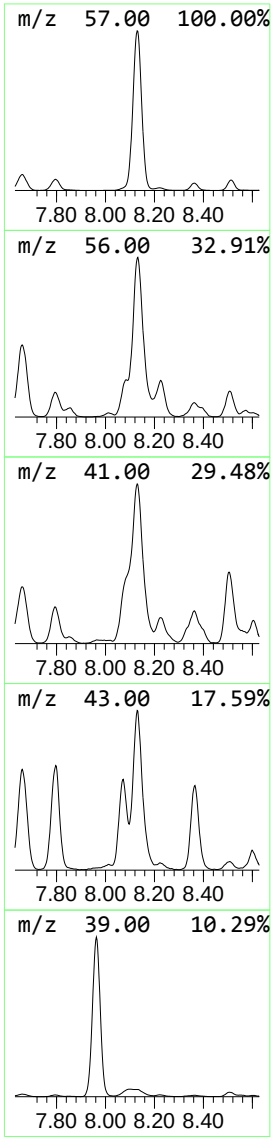
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.129	79.67 ug/l	5843360	1,4-Difluorobenzene	8.512

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
2	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	64
3	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	64
4	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	53
5	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	53





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Data File : VN066381.D
Acq On : 29 Mar 2021 16:58
Operator : JC/MD
Sample : M1835-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ASR4

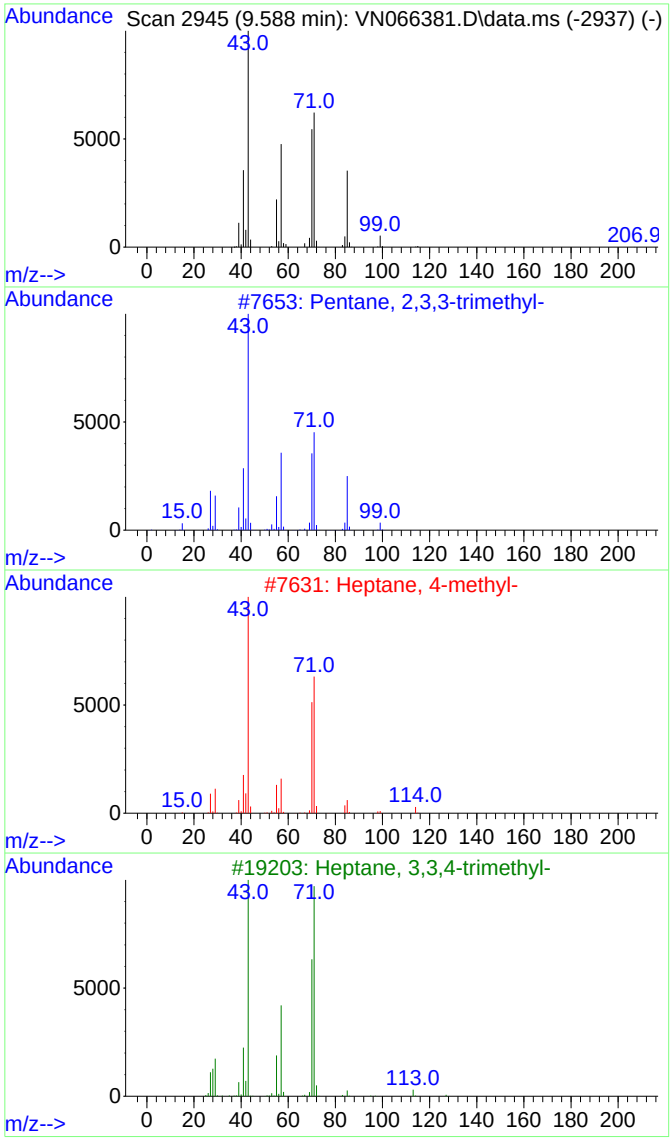
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

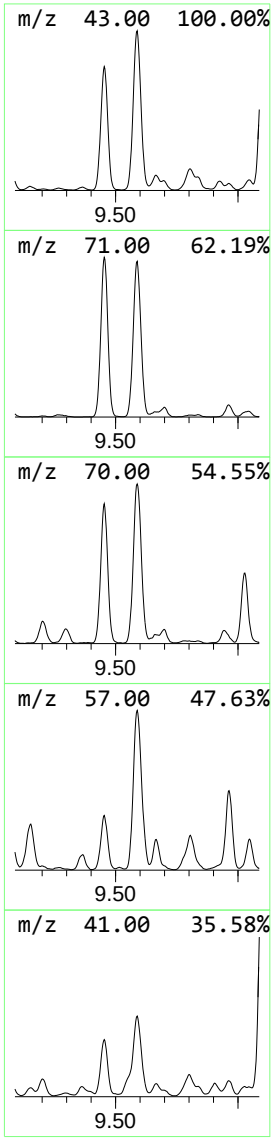
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Pentane, 2,3,3-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.588	41.09 ug/l	3013700	1,4-Difluorobenzene	8.512

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	80
2	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3	Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	59
4	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59
5	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032921\
Data File : VN066381.D
Acq On : 29 Mar 2021 16:58
Operator : JC/MD
Sample : M1835-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ASR4

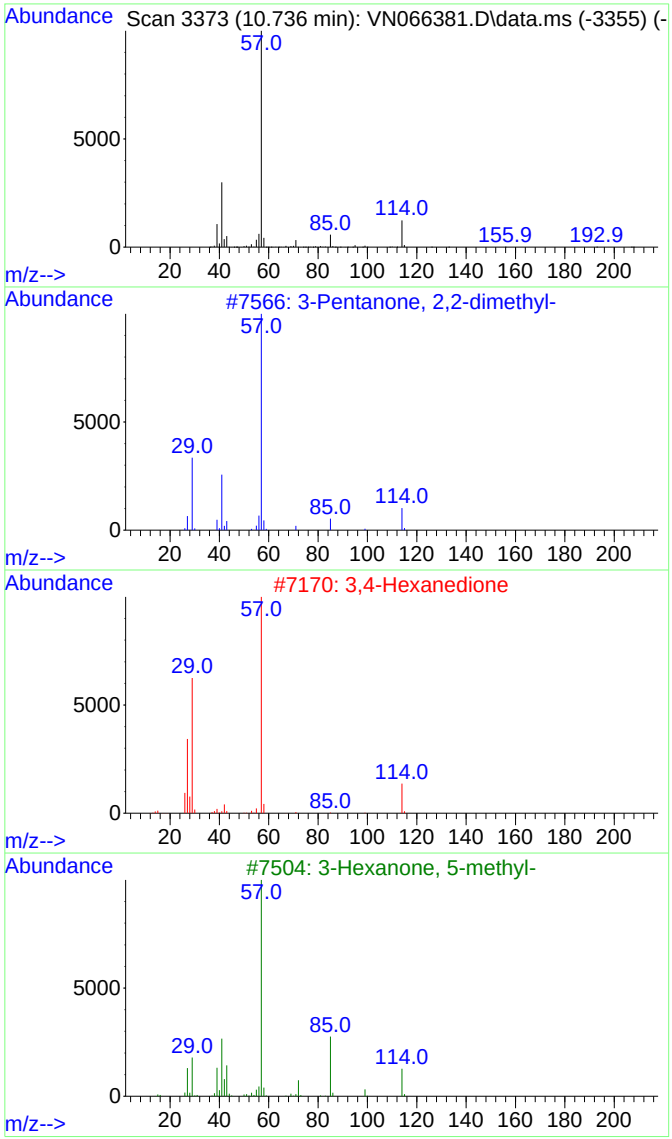
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

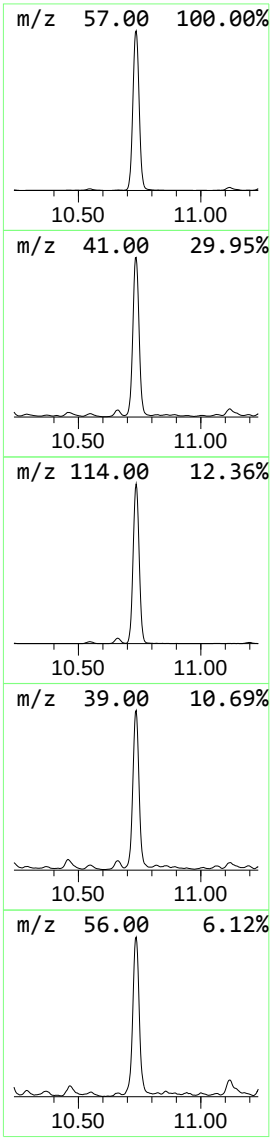
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 3-Pentanone, 2,2-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.736	168.12 ug/l	8104860	Chlorobenzene-d5	11.350

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,2-dimethyl-	114	C7H14O	000564-04-5	86
2	3,4-Hexanedione	114	C6H10O2	004437-51-8	58
3	3-Hexanone, 5-methyl-	114	C7H14O	000623-56-3	53
4	3-Heptanone	114	C7H14O	000106-35-4	42
5	2,2,5,5-Tetramethyl-3-hexanone	156	C10H20O	000868-91-7	42





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Data File : VN066381.D
Acq On : 29 Mar 2021 16:58
Operator : JC/MD
Sample : M1835-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ASR4

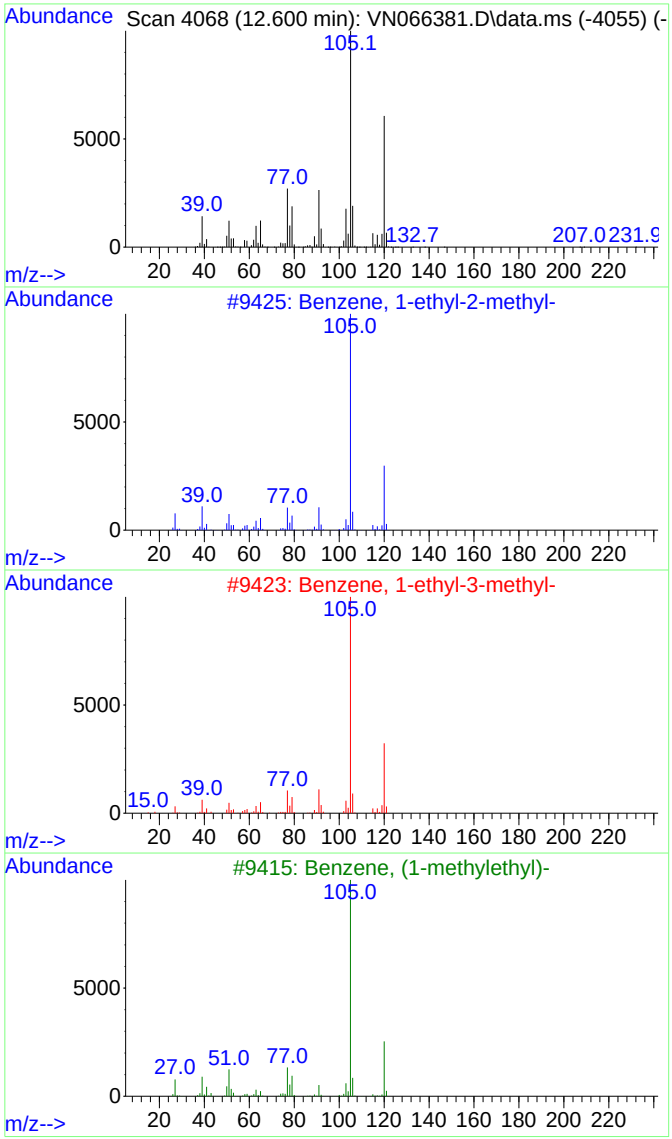
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

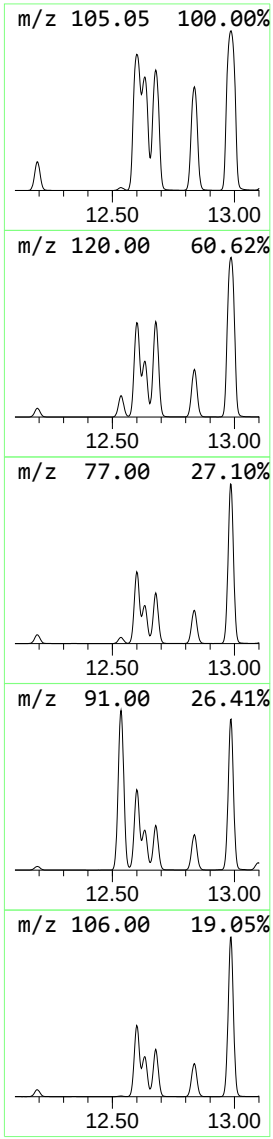
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.600	60.45 ug/l	34548200	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	87
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	81
3	Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	68
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	64
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032921\
Data File : VN066381.D
Acq On : 29 Mar 2021 16:58
Operator : JC/MD
Sample : M1835-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ASR4

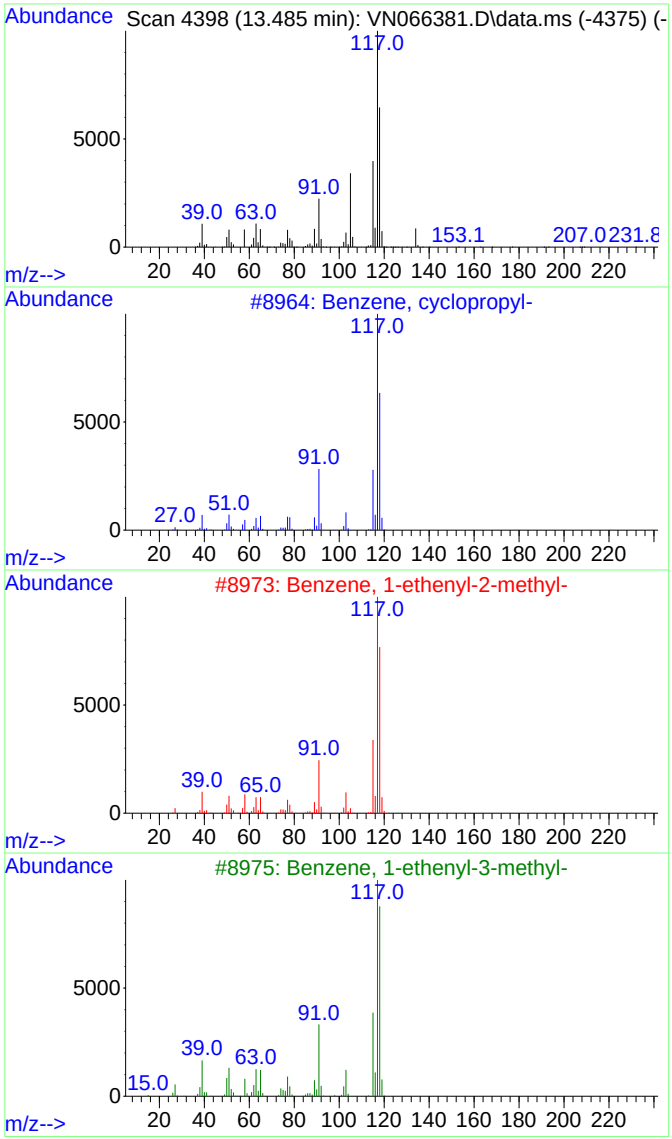
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

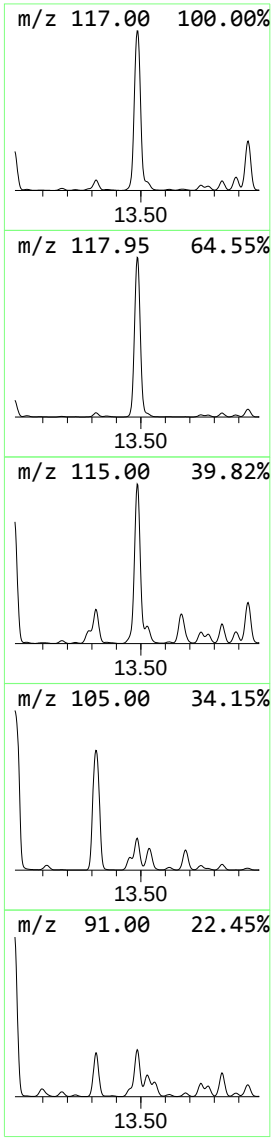
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, cyclopropyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.485	44.89 ug/l	25656300	1,4-Dichlorobenzene-d4	13.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, cyclopropyl-	118	C9H10	000873-49-4	92
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	91
3	Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	86
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	83
5	Indane	118	C9H10	000496-11-7	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032921\
Data File : VN066381.D
Acq On : 29 Mar 2021 16:58
Operator : JC/MD
Sample : M1835-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : ASR4

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-methyl-	2.752	44.9	ug/l	3115970	1	7.585	3472680	50.0
Cyclopropane, e...	3.087	36.2	ug/l	2512180	1	7.585	3472680	50.0
Cyclopropane, 1...	3.492	91.6	ug/l	6362270	1	7.585	3472680	50.0
Cyclopentene	4.329	40.1	ug/l	2783740	1	7.585	3472680	50.0
Cyclopentane, m...	6.525	52.0	ug/l	3612950	1	7.585	3472680	50.0
Pentane, 2,2,4-...	8.129	79.7	ug/l	5843360	2	8.512	3667380	50.0
Pentane, 2,3,3-...	9.588	41.1	ug/l	3013700	2	8.512	3667380	50.0
3-Pentanone, 2,...	10.736	168.1	ug/l	8104860	3	11.350	2410440	50.0
Benzene, 1-ethy...	12.600	60.5	ug/l	34548200	4	13.286	28578000	50.0
Benzene, cyclop...	13.485	44.9	ug/l	25656300	4	13.286	28578000	50.0