LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080322\
Data File : VN073717.D
Acq On : 03 Aug 2022 17:28
Operator : JC\MD
Sample : N3972-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-9

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\82N072822W.M
Title : SW846 8260

Signal : TIC: VN073717.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.205	48	54	56	rBV	12179	22808	1.35%	0.173%
2	2.399	80	87	92	rBV	30697	48134	2.84%	0.365%
3	2.705	133	139	140	rBV4	12448	21737	1.28%	0.165%
4	3.081	195	203	219	rVB	311317	692881	40.89%	5.259%
5	3.452	256	266	276	rVB3	12211	30297	1.79%	0.230%
6	3.922	337	346	358	rBV3	13143	36823	2.17%	0.280%
7	4.234	392	399	410	rVB	22053	62799	3.71%	0.477%
8	4.510	437	446	464	rBV2	74016	233080	13.75%	1.769%
9	4.998	515	529	536	rBV5	30803	120996	7.14%	0.918%
10	5.104	536	547	562	rVB3	48429	197890	11.68%	1.502%
11	5.528	609	619	633	rBV5	15223	52671	3.11%	0.400%
12	6.387	755	765	775	rBV7	6223	20958	1.24%	0.159%
13	6.516	778	787	799	rBV6	8487	26985	1.59%	0.205%
14	7.069	869	881	889	rBV2	61603	188978	11.15%	1.434%
15	7.145	889	894	906	rVB4	18851	46414	2.74%	0.352%
16	7.345	920	928	946	rVB	54091	137551	8.12%	1.044%
17	7.628	962	976	983	rBV4	10255	29933	1.77%	0.227%
18	7.951	1020	1031	1037	rBV	261374	656545	38.74%	4.984%
19	8.016	1037	1042	1054	rVV	474284	1092091	64.44%	8.290%
20	8.375	1093	1103	1115	rBV	266528	647234	38.19%	4.913%
21	8.904	1181	1193	1217	rBV	634777	1323734	78.11%	10.048%
22	9.910	1358	1364	1369	rBV2	13988	24028	1.42%	0.182%
23	10.139	1395	1403	1418	rBV6	6966	21792	1.29%	0.165%
24	10.380	1436	1444	1453	rBV	928857	1694625	100.00%	12.863%
25	10.586	1471	1479	1485	rBV	131590	243828	14.39%	1.851%
26	10.657	1485	1491	1500	rVB	148785	259150	15.29%	1.967%
27	11.239	1581	1590	1599	rBV2	29352	58466	3.45%	0.444%
28	11.686	1657	1666	1678	rBV	925628	1625328	95.91%	12.337%
29	11.898	1694	1702	1711	rVB	16938	30634	1.81%	0.233%
30	12.522	1797	1808	1815	rBV	64204	115991	6.84%	0.880%
31	12.674	1826	1834	1846	rBV	759945	1283392	75.73%	9.742%
32	12.863	1860	1866	1872	rBV	75203	122554	7.23%	0.930%
33	13.616	1987	1994	2006	rBV	957509	1590209	93.84%	12.071%
34	13.710	2006	2010	2016	rVV	46691	76906	4.54%	0.584%
35	13.816	2023	2028	2045	rVB	151512	262908	15.51%	1.996%
36	14.268	2099	2105	2112	rBV2	18347	30210	1.78%	0.229%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080322\
Data File : VN073717.D
Acq On : 03 Aug 2022 17:28
Operator : JC\MD
Sample : N3972-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-9

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\82N072822W.M
Title : SW846 8260

37	14.751	2182	2187	2194	rBV3	10143	18689	1.10%	0.142%
38	14.874	2201	2208	2214	rVB5	13261	24871	1.47%	0.189%

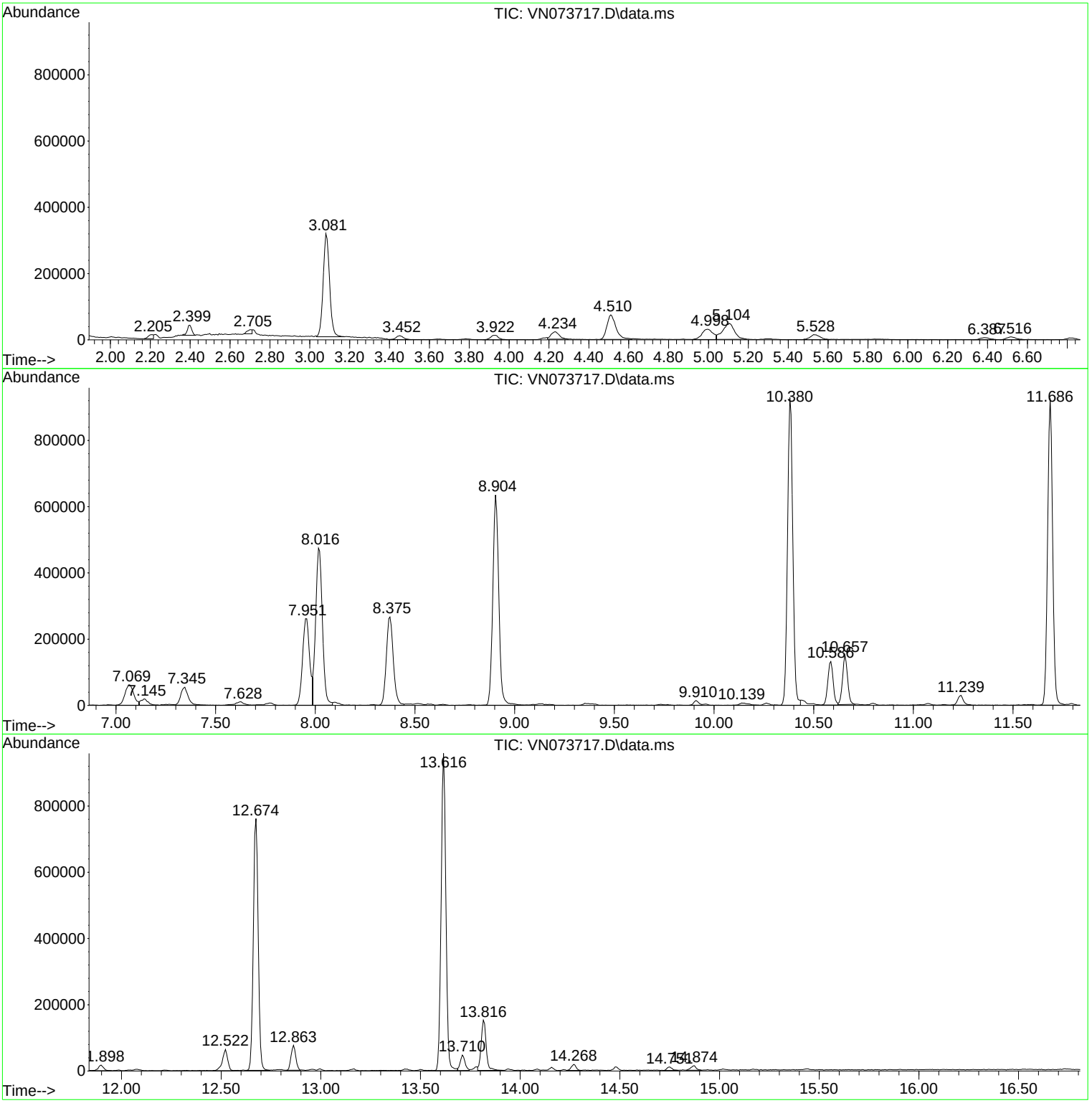
Sum of corrected areas: 13174120

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080322\
Data File : VN073717.D
Acq On : 03 Aug 2022 17:28
Operator : JC\MD
Sample : N3972-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080322\
Data File : VN073717.D
Acq On : 03 Aug 2022 17:28
Operator : JC\MD
Sample : N3972-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-9

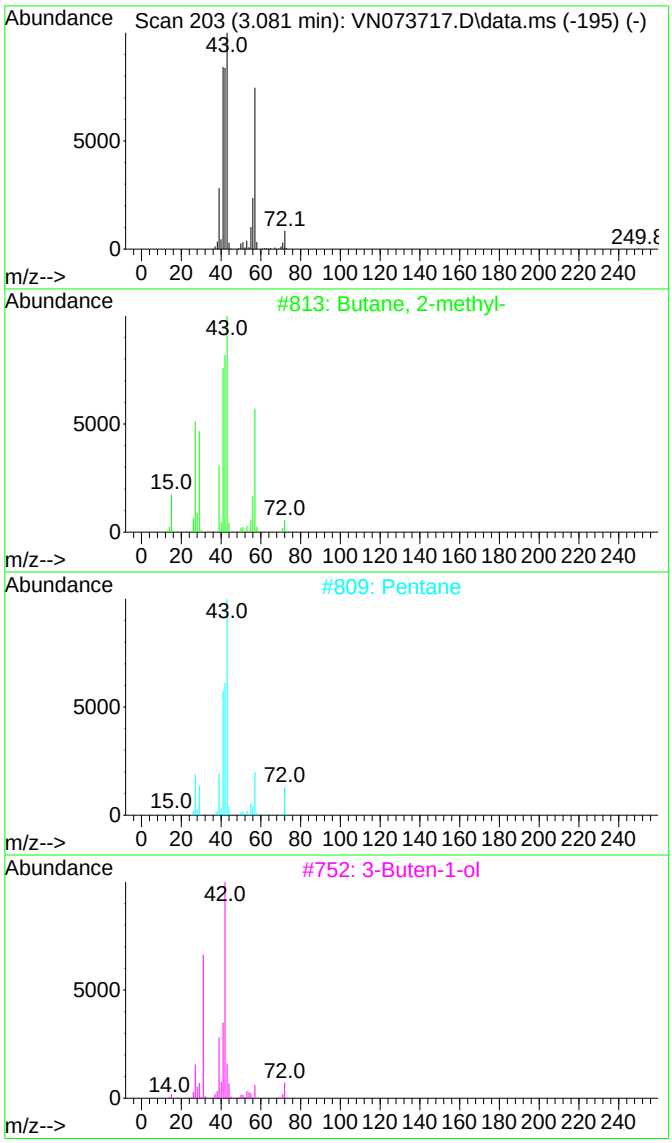
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

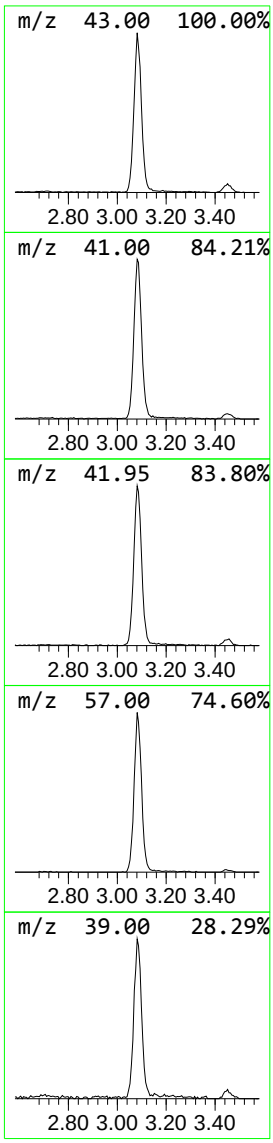
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.081	31.72 ug/l	692881	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2	Pentane	72	C5H12	000109-66-0	38
3	3-Buten-1-ol	72	C4H8O	000627-27-0	28
4	1-Propene, 2-methyl-	56	C4H8	000115-11-7	14
5	1-Butene	56	C4H8	000106-98-9	14





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080322\
Data File : VN073717.D
Acq On : 03 Aug 2022 17:28
Operator : JC\MD
Sample : N3972-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-9

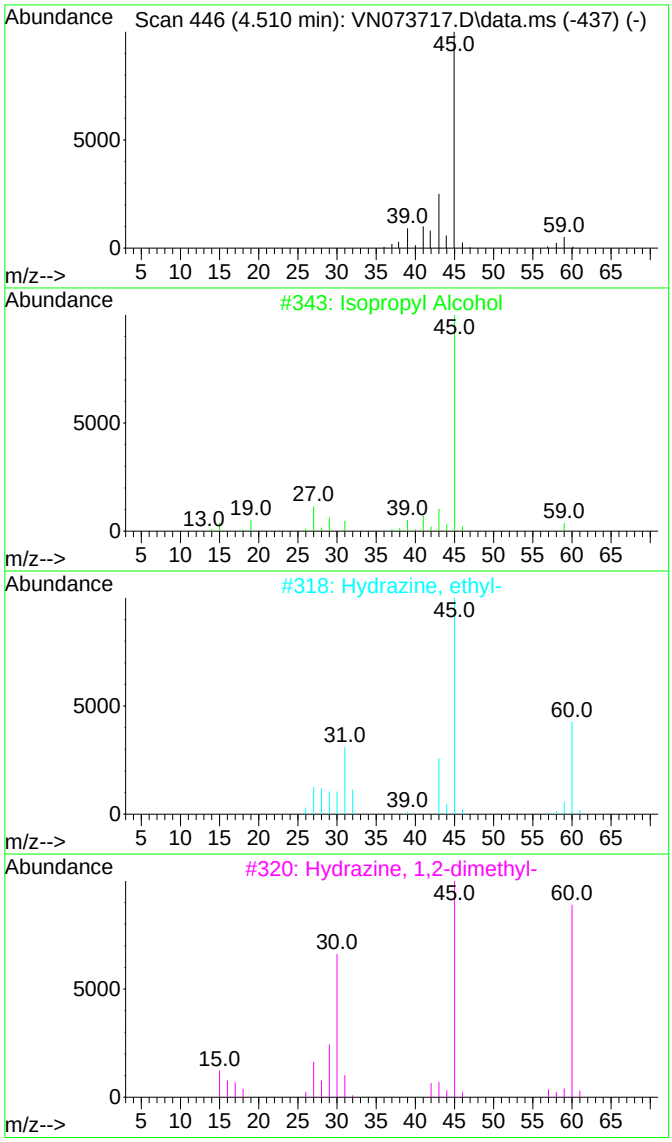
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

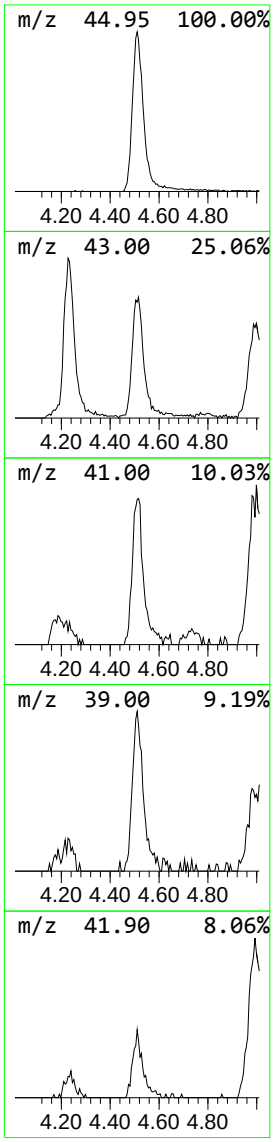
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Isopropyl Alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.510	10.67 ug/l	233080	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2	Hydrazine, ethyl-	60	C2H8N2	000624-80-6	40
3	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4	4-Penten-2-ol	86	C5H10O	000625-31-0	9
5	Ethylamine	45	C2H7N	000075-04-7	5





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080322\
Data File : VN073717.D
Acq On : 03 Aug 2022 17:28
Operator : JC\MD
Sample : N3972-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-9

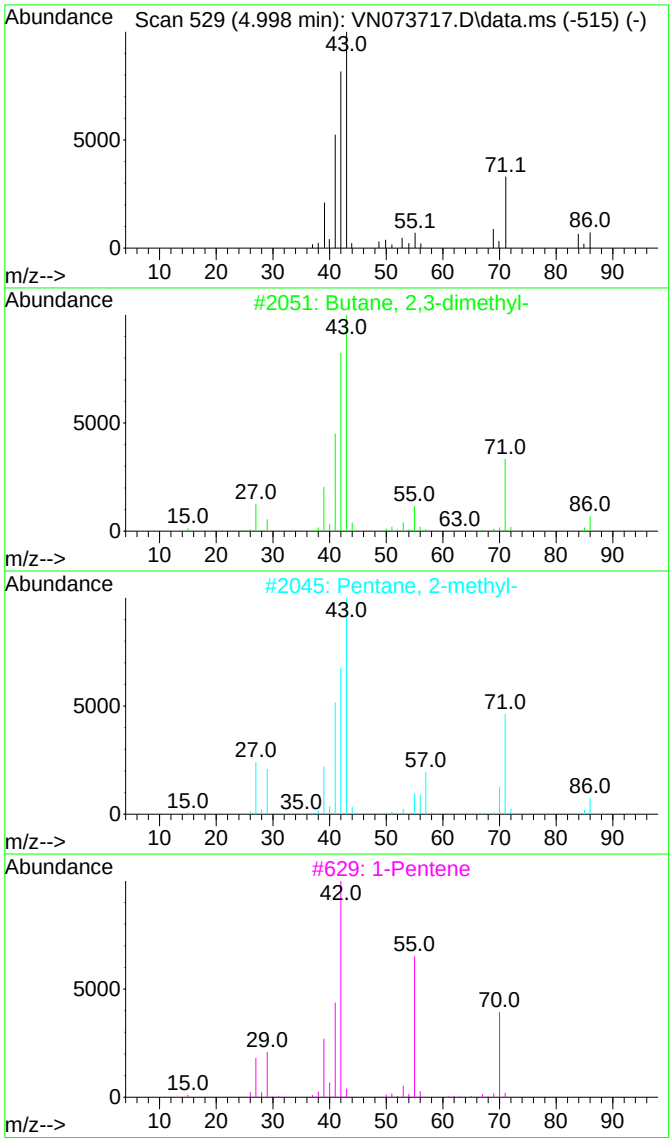
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

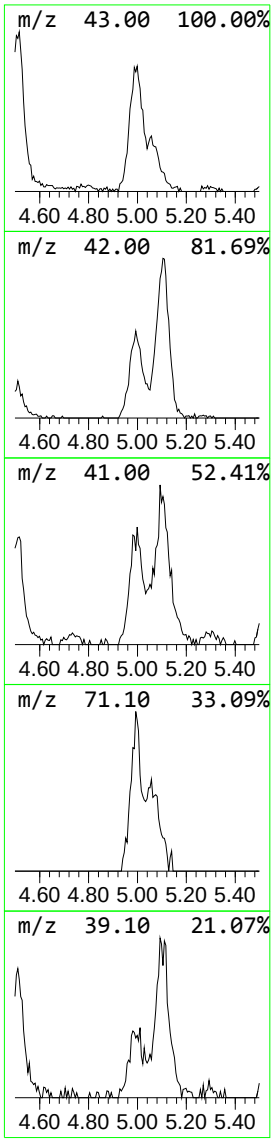
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butane, 2,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.998	5.54 ug/l	120996	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	45
3	1-Pentene	70	C5H10	000109-67-1	28
4	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	9
5	1,2,3-Trimethyldiaziridine	86	C4H10N2	113604-56-1	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080322\
Data File : VN073717.D
Acq On : 03 Aug 2022 17:28
Operator : JC\MD
Sample : N3972-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-9

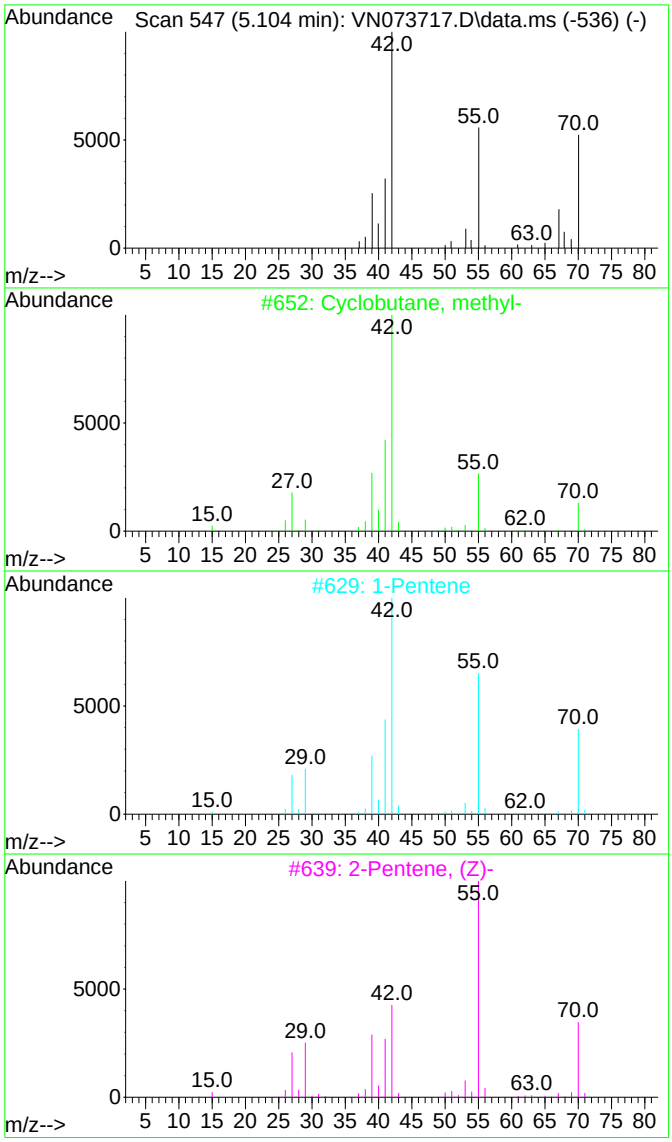
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

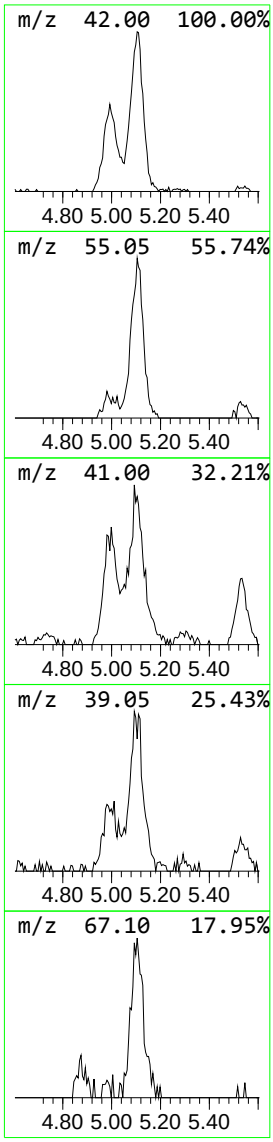
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclobutane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	9.06 ug/l	197890	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, methyl-	70	C5H10	000598-61-8	72
2	1-Pentene	70	C5H10	000109-67-1	64
3	2-Pentene, (Z)-	70	C5H10	000627-20-3	47
4	2-Pentene	70	C5H10	000109-68-2	47
5	2-Pentene, (E)-	70	C5H10	000646-04-8	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080322\
Data File : VN073717.D
Acq On : 03 Aug 2022 17:28
Operator : JC\MD
Sample : N3972-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-9

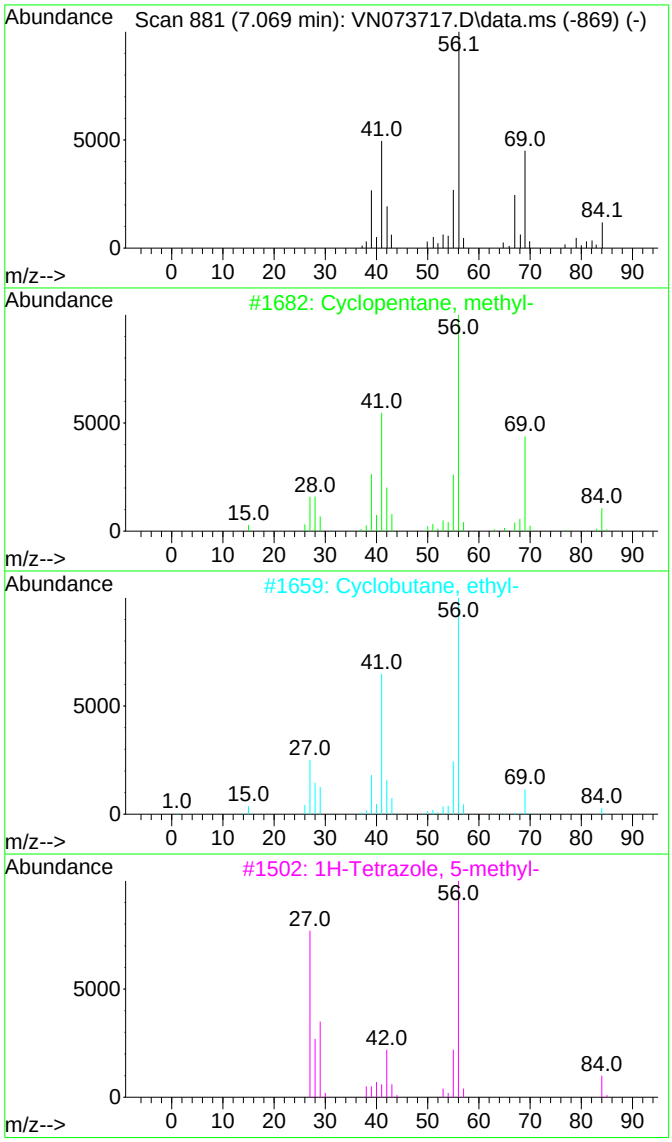
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

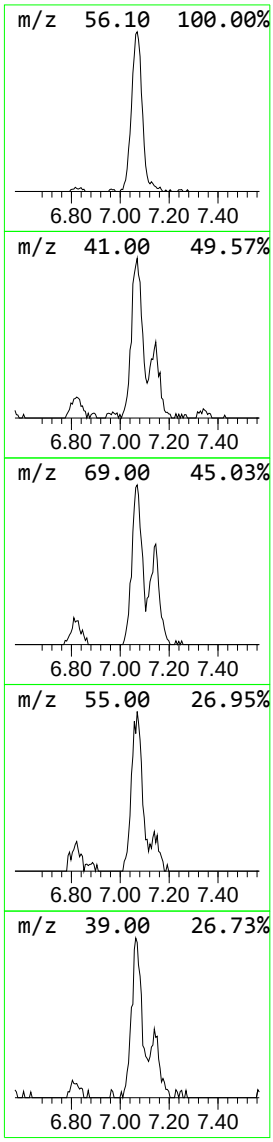
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.069	8.65 ug/l	188978	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	81
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	59
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	50
4	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	50
5	Cyclobutane, butyl-	112	C8H16	013152-44-8	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080322\
Data File : VN073717.D
Acq On : 03 Aug 2022 17:28
Operator : JC\MD
Sample : N3972-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-9

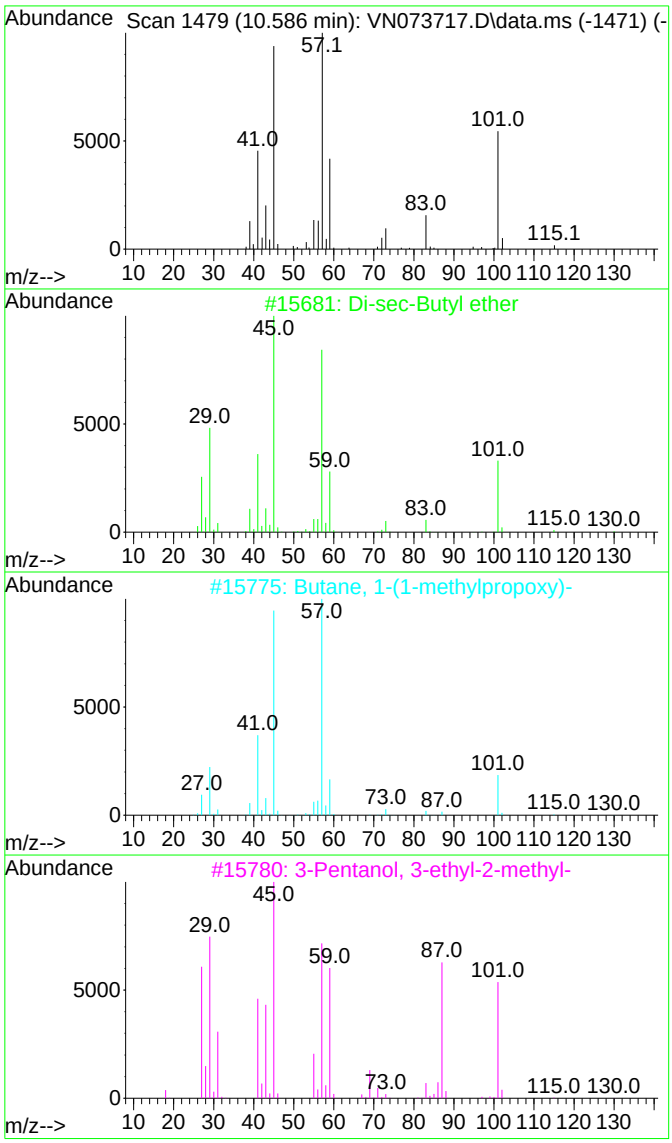
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

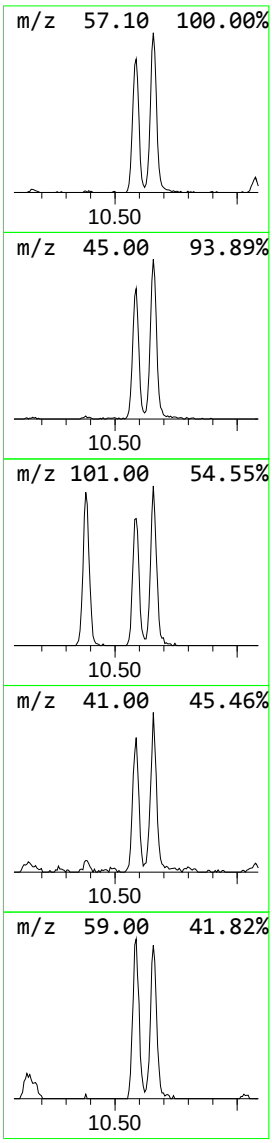
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Di-sec-Butyl ether Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.586	7.50 ug/l	243828	Chlorobenzene-d5	11.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	83
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	64
3	3-Pentanol, 3-ethyl-2-methyl-	130	C8H18O	000597-05-7	64
4	Sulfurous acid, isobutyl 2-methy...	238	C10H22O4S	1000309-20-3	50
5	trans-2-Hexenyl lactate	172	C9H16O3	1000431-56-9	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080322\
Data File : VN073717.D
Acq On : 03 Aug 2022 17:28
Operator : JC\MD
Sample : N3972-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-9

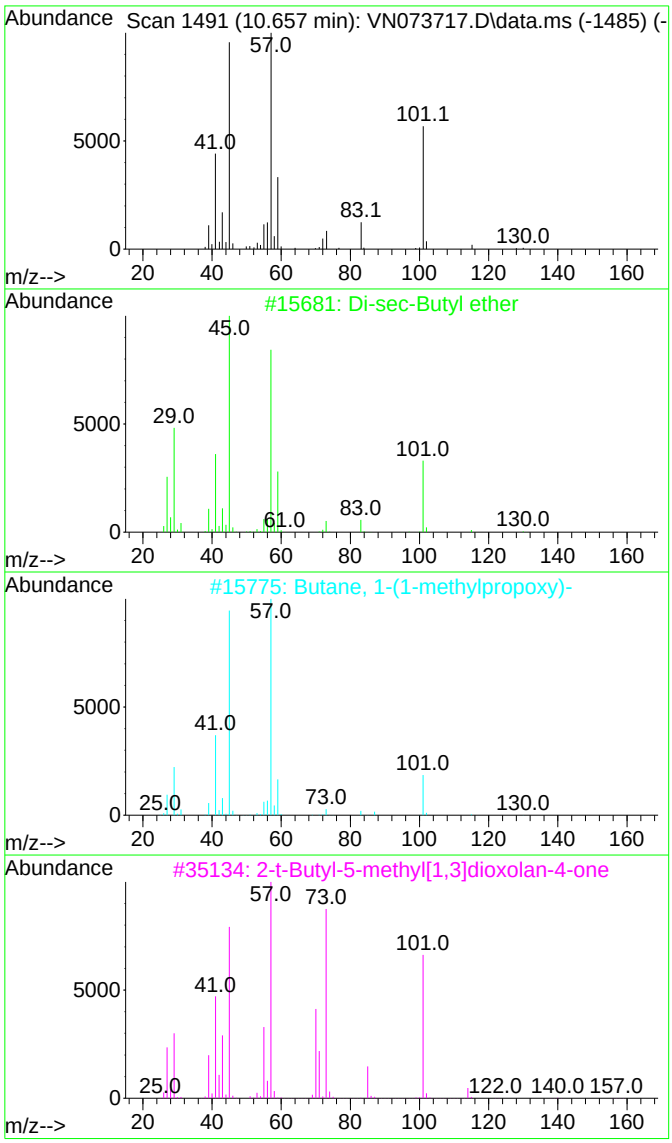
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

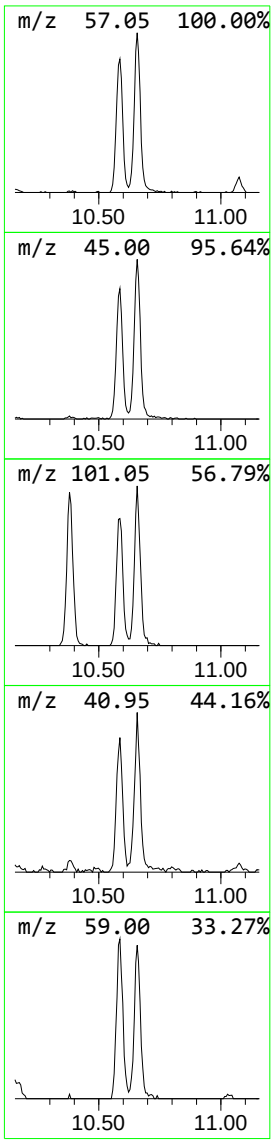
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Butane, 1-(1-methylpropoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.657	7.97 ug/l	259150	Chlorobenzene-d5	11.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	91
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
3	2-t-Butyl-5-methyl[1,3]dioxolan-...	158	C8H14O3	130930-47-1	50
4	DL-Lactamide, butyl ether	145	C7H15NO2	1000452-56-5	50
5	Sulfurous acid, isobutyl 2-methy...	238	C10H22O4S	1000309-20-3	45





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080322\
Data File : VN073717.D
Acq On : 03 Aug 2022 17:28
Operator : JC\MD
Sample : N3972-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-9

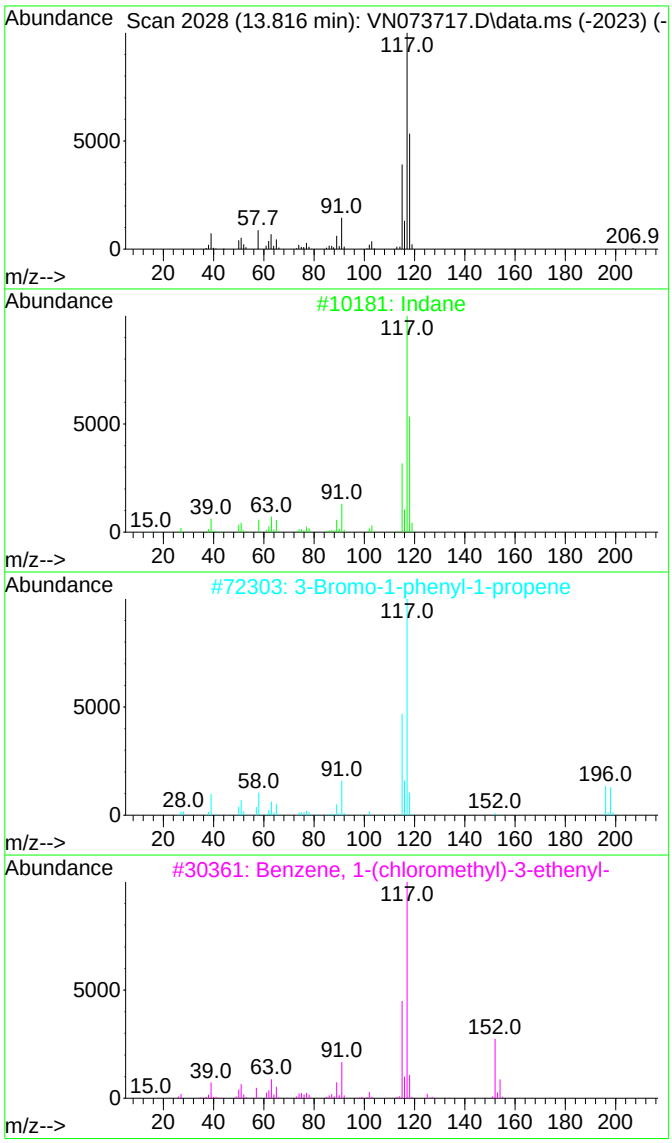
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

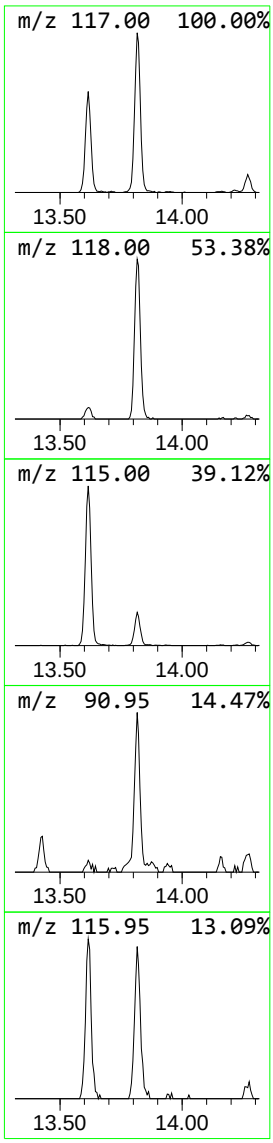
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Indane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	8.27 ug/l	262908	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	89
2	3-Bromo-1-phenyl-1-propene	196	C9H9Br	004392-24-9	64
3	Benzene, 1-(chloromethyl)-3-ethe...	152	C9H9Cl	039833-65-3	59
4	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	59
5	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080322\
Data File : VN073717.D
Acq On : 03 Aug 2022 17:28
Operator : JC\MD
Sample : N3972-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SPN-9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.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
Butane, 2-methyl-	3.081	31.7	ug/l	692881	1	8.016	1092090	50.0
Isopropyl Alcohol	4.510	10.7	ug/l	233080	1	8.016	1092090	50.0
Butane, 2,3-dim...	4.998	5.5	ug/l	120996	1	8.016	1092090	50.0
Cyclobutane, me...	5.104	9.1	ug/l	197890	1	8.016	1092090	50.0
Cyclopentane, m...	7.069	8.7	ug/l	188978	1	8.016	1092090	50.0
Di-sec-Butyl ether	10.586	7.5	ug/l	243828	3	11.686	1625330	50.0
Butane, 1-(1-me...	10.657	8.0	ug/l	259150	3	11.686	1625330	50.0
Indane	13.816	8.3	ug/l	262908	4	13.616	1590210	50.0