LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032024\
Data File : VN081500.D
Acq On : 20 Mar 2024 17:46
Operator : JC\MD
Sample : P1799-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
50296

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\82N031824W.M
Title : SW846 8260

Signal : TIC: VN081500.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.512	84	95	107	rBV	4915081	9103941	5.63%	1.949%
2	2.665	117	121	129	rVV	1625162	2822717	1.75%	0.604%
3	3.248	210	220	232	rBV	1593419	3566676	2.21%	0.764%
4	3.653	279	289	301	rBV2	762695	2548061	1.58%	0.546%
5	3.824	301	318	338	rBV2	20324622	65533378	40.54%	14.031%
6	4.147	363	373	390	rVB	1382066	3880217	2.40%	0.831%
7	5.159	529	545	557	rBV	707232	2373101	1.47%	0.508%
8	5.383	569	583	604	rVB3	407643	1715409	1.06%	0.367%
9	5.794	638	653	672	rBV2	1341853	4723706	2.92%	1.011%
10	6.671	791	802	815	rVB2	712525	2247985	1.39%	0.481%
11	7.559	945	953	968	rVB	1617554	3949620	2.44%	0.846%
12	8.230	1061	1067	1081	rVB2	820059	2495700	1.54%	0.534%
13	8.612	1119	1132	1148	rBV2	46342161	111345362	68.89%	23.839%
14	9.100	1205	1215	1235	rBV	1081742	2300987	1.42%	0.493%
15	10.571	1457	1465	1469	rBV	1551473	3024632	1.87%	0.648%
16	10.635	1469	1476	1505	rVB2	77555860	161636889	100.00%	34.606%
17	11.865	1677	1685	1693	rBV	1433536	2575642	1.59%	0.551%
18	11.965	1693	1702	1711	rVV	7153388	11727302	7.26%	2.511%
19	12.070	1711	1720	1733	rVV	19660279	37200766	23.02%	7.965%
20	12.400	1767	1776	1784	rBV	10211668	16976757	10.50%	3.635%
21	12.853	1845	1853	1861	rVB	1130775	1974258	1.22%	0.423%
22	13.100	1889	1895	1899	rBV	1874590	3271263	2.02%	0.700%
23	13.482	1951	1960	1971	rBV	3217972	5278213	3.27%	1.130%
24	13.794	2006	2013	2016	rBV	1430103	2690496	1.66%	0.576%
25	13.994	2041	2047	2063	rVB3	823784	2113990	1.31%	0.453%

Sum of corrected areas: 467077068

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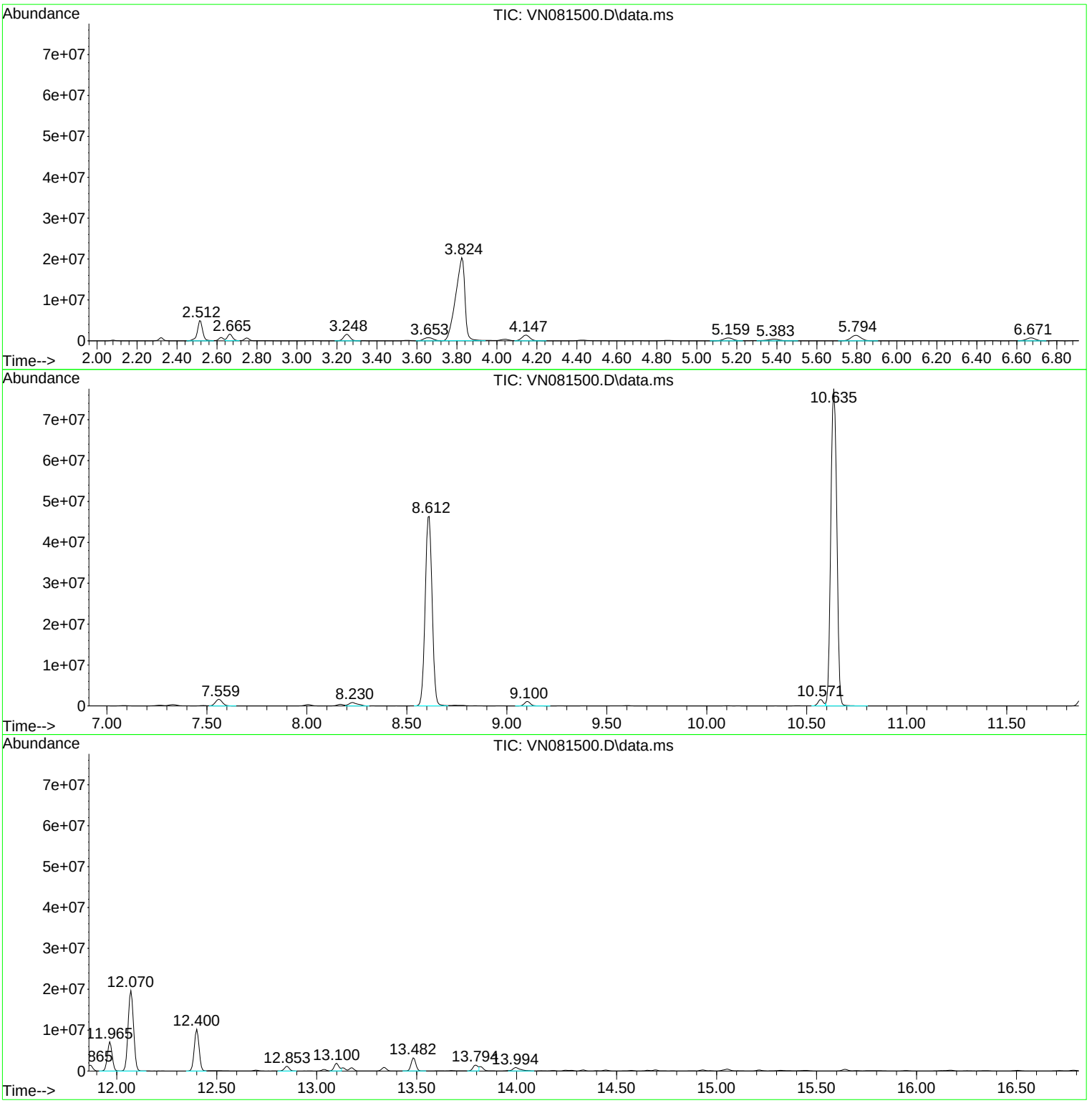
50296

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

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



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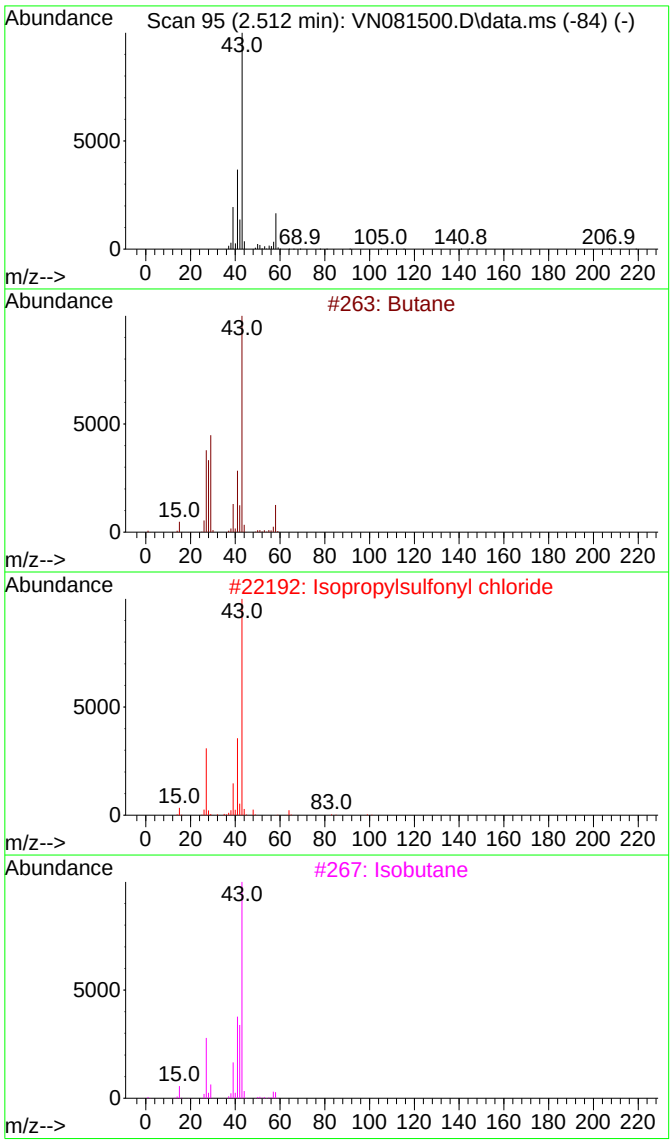
Quant Title : SW846 8260

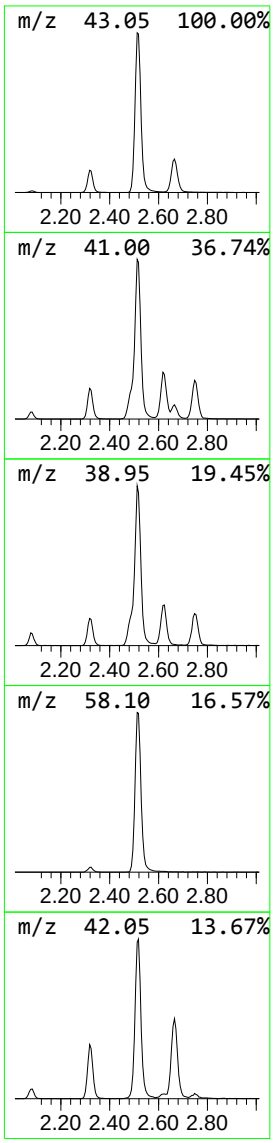
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.512	182.39 ug/l	9103940	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	80
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	Acetone	58	C3H6O	000067-64-1	7





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ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

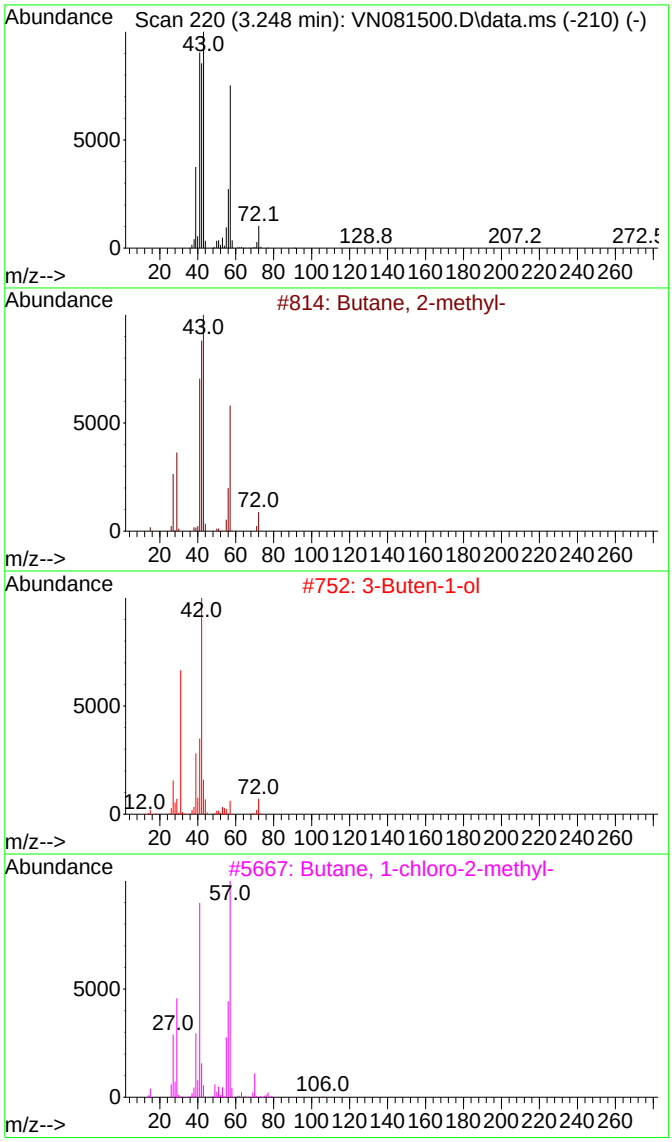
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

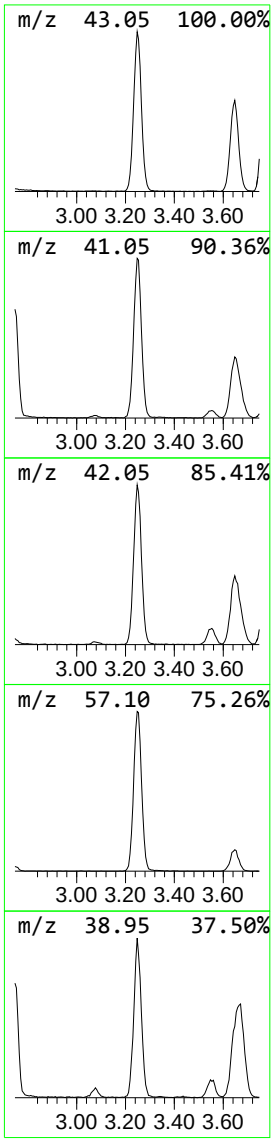
****

Peak Number 3 Butane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.248	71.46 ug/l	3566680	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2	3-Buten-1-ol	72	C4H8O	000627-27-0	43
3	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	35
4	Oxirane, trimethyl-	86	C5H10O	005076-19-7	33
5	Pentane	72	C5H12	000109-66-0	28





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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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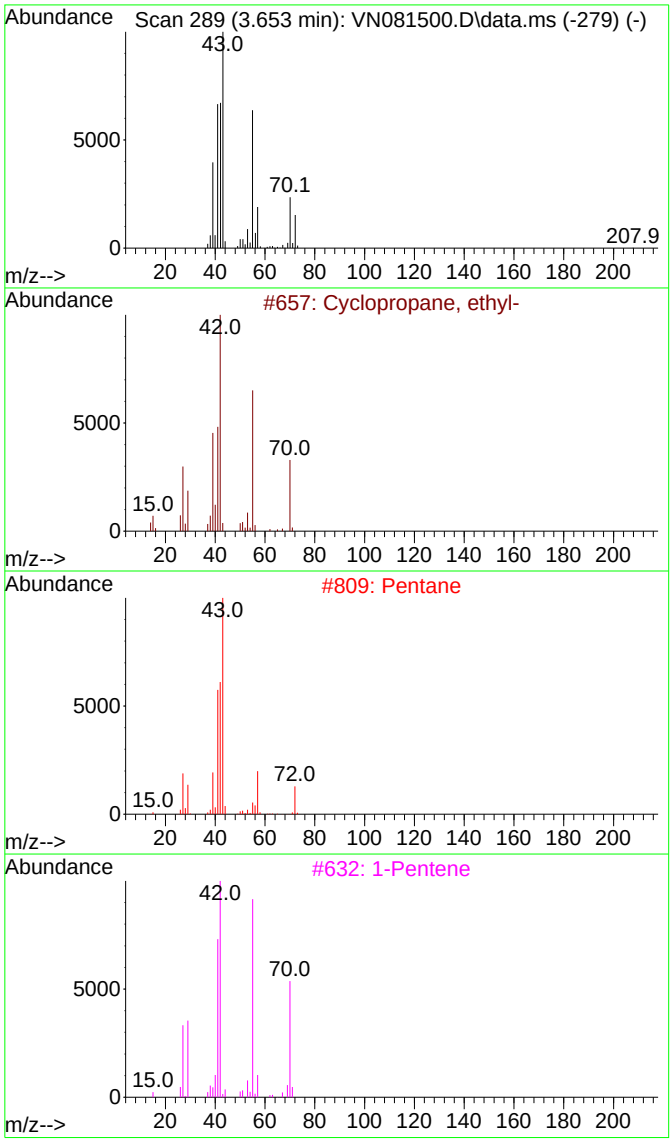
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

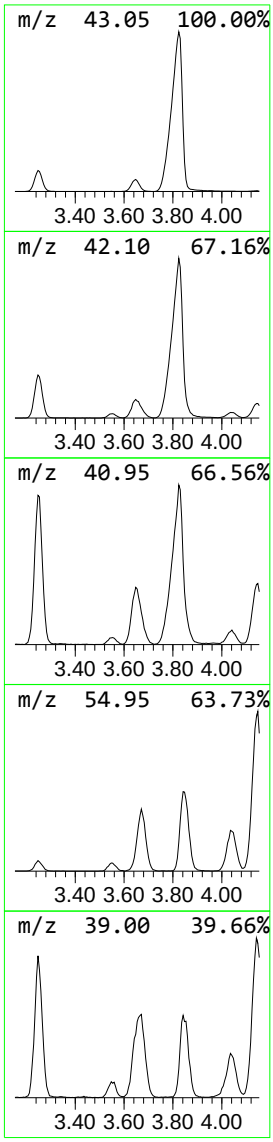
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopropane, ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.653	51.05 ug/l	2548060	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, ethyl-	70	C5H10	001191-96-4	58
2	Pentane	72	C5H12	000109-66-0	49
3	1-Pentene	70	C5H10	000109-67-1	46
4	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	38
5	2-Pentene, (Z)-	70	C5H10	000627-20-3	27





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Instrument :
MSVOA_N
ClientSampleId :
50296

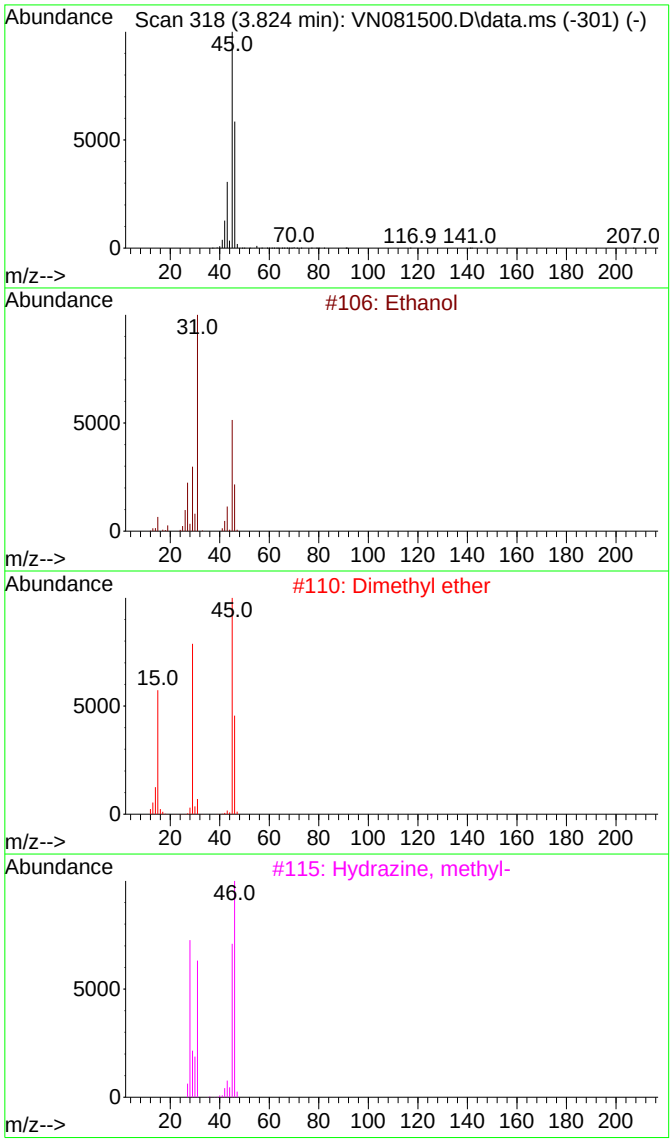
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

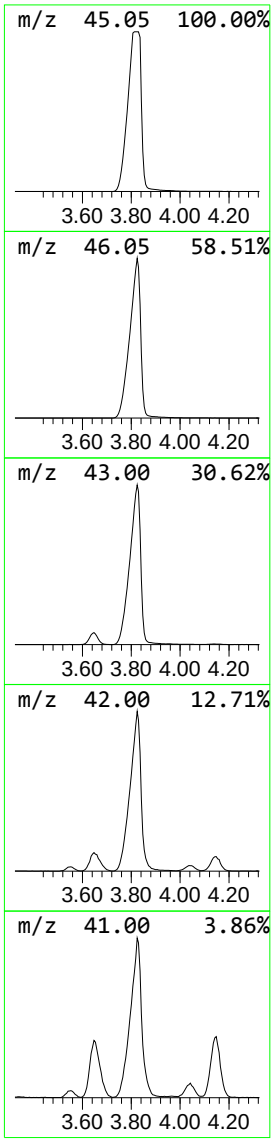
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.824	1312.93 ug/l	65533400	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	56
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Hydrazine, methyl-	46	CH6N2	000060-34-4	9
4	Methane, nitroso-	45	CH3NO	000865-40-7	4
5	Ethene, fluoro-	46	C2H3F	000075-02-5	4





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Instrument :
MSVOA_N
ClientSampleId :
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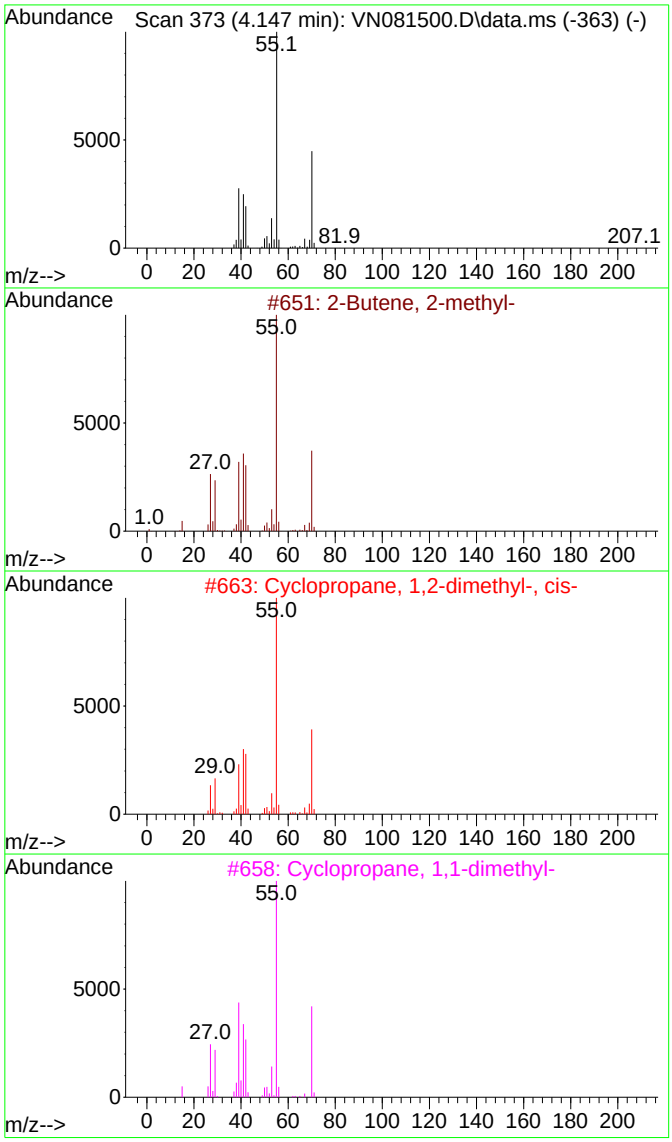
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

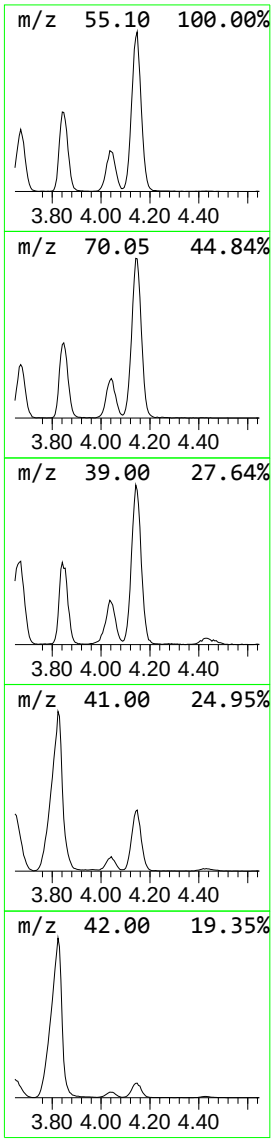
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Butene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.147	77.74 ug/l	3880220	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene, 2-methyl-	70	C5H10	000513-35-9	90
2	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	86
3	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80
4	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	74
5	1-Butene, 3-methyl-	70	C5H10	000563-45-1	72





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Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

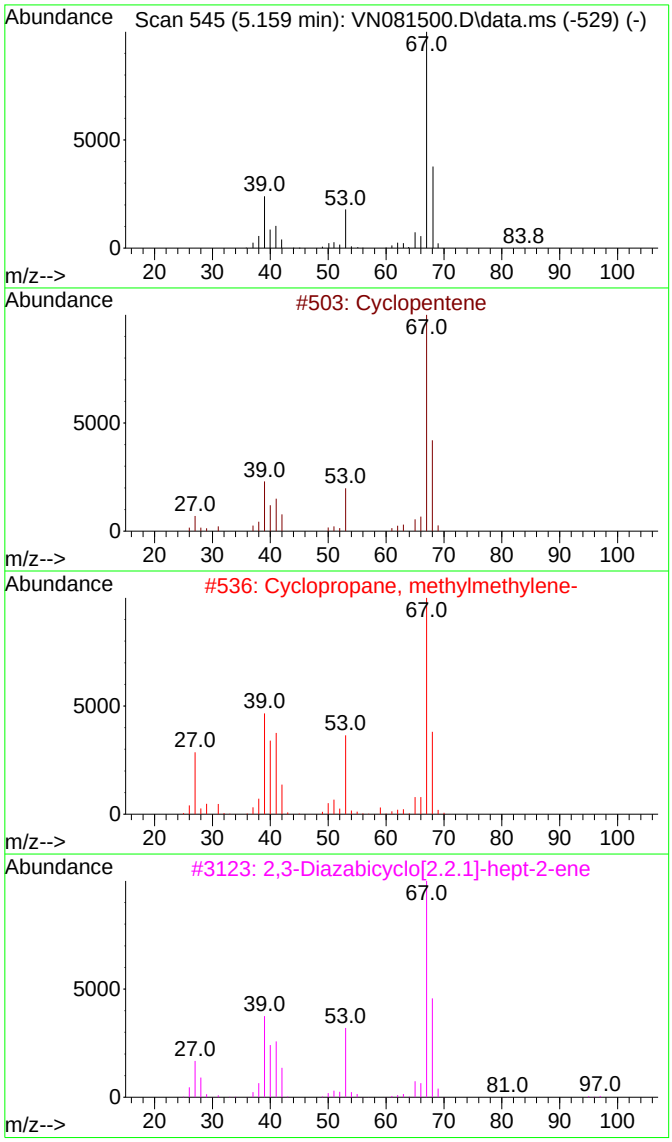
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

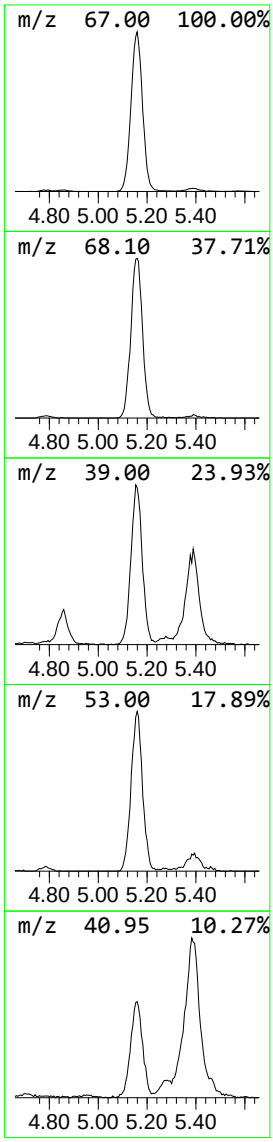
****

Peak Number 7 Cyclopentene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.159	47.54 ug/l	2373100	Pentafluorobenzene	8.224

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	64
4	Bicyclo[2.1.0]pentane	68	C5H8	000185-94-4	59
5	1,3-Pentadiene, (E)-	68	C5H8	002004-70-8	53





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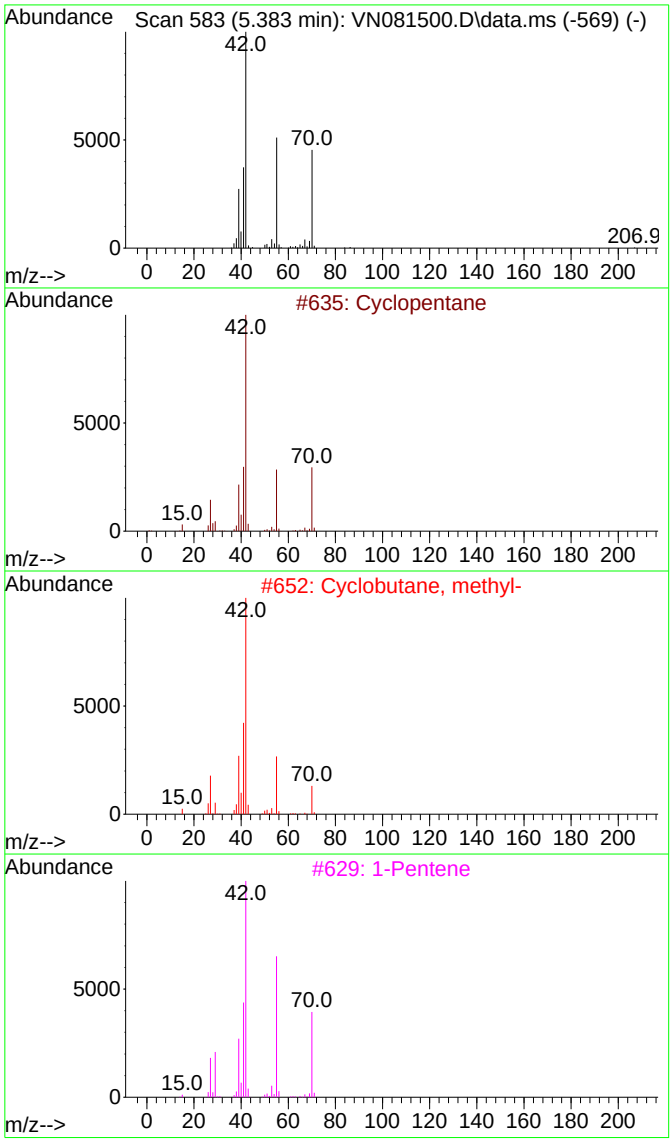
Quant Title : SW846 8260

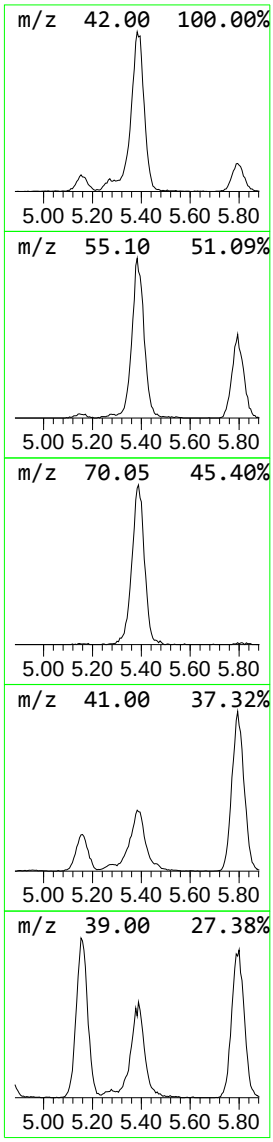
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Cyclobutane, methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.383	34.37 ug/l	1715410	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	78
2	Cyclobutane, methyl-	70	C5H10	000598-61-8	78
3	1-Pentene	70	C5H10	000109-67-1	64
4	2-Pentene, (Z)-	70	C5H10	000627-20-3	47
5	2-Pentene	70	C5H10	000109-68-2	47





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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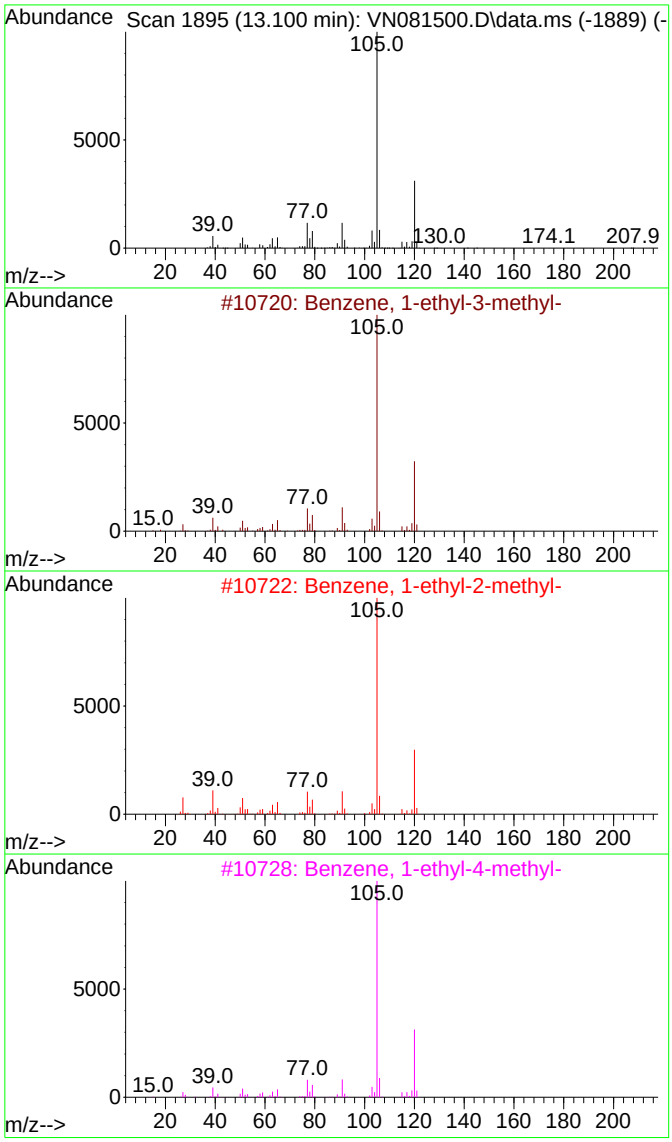
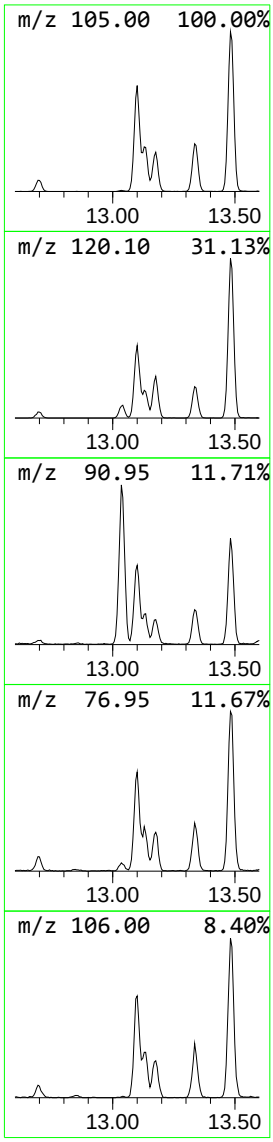
****
Peak Number 9 Benzene, 1-ethyl-3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	60.79 ug/l	3271260	1,4-Dichlorobenzene-d4	13.794

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





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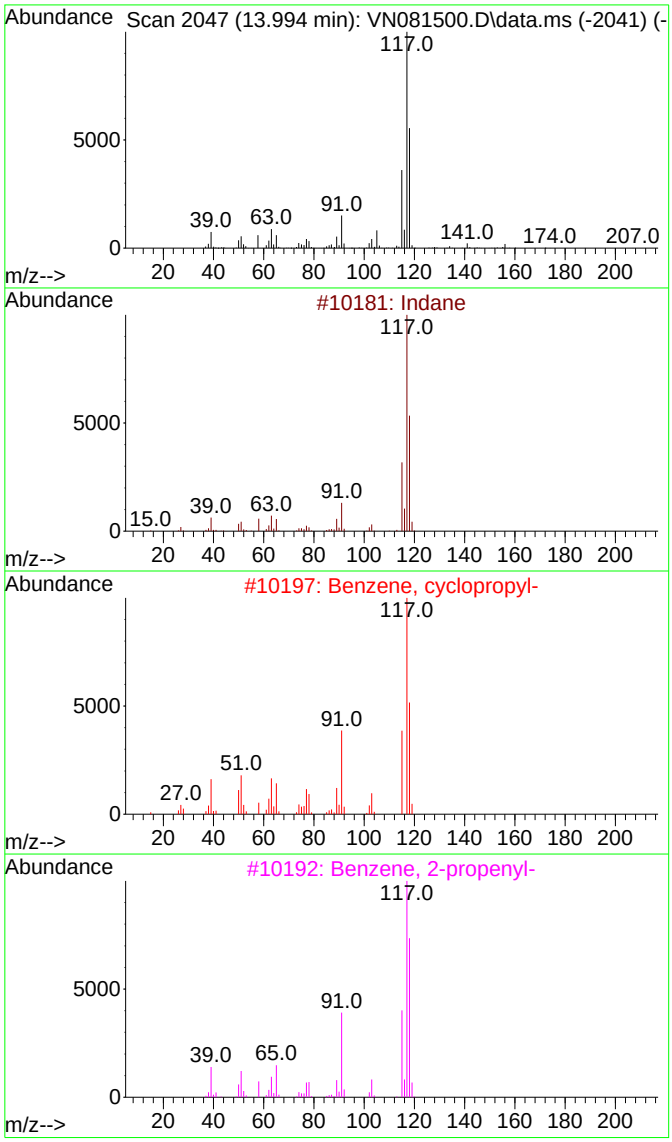
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

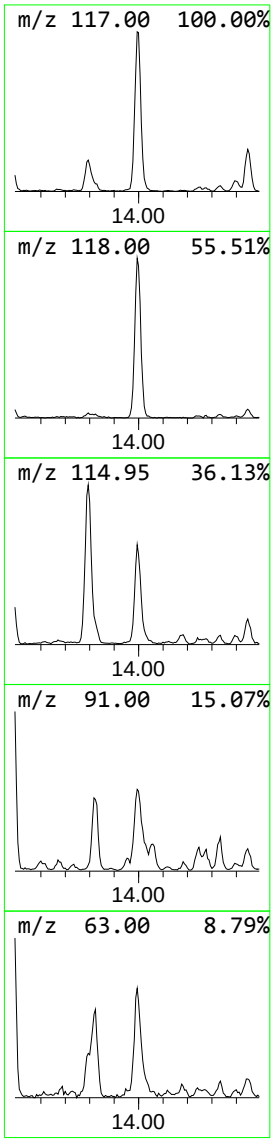
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Indane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	39.29 ug/l	2113990	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	91
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
4	Benzene, 1-propenyl-	118	C9H10	000637-50-3	74
5	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	68





Tentatively Identified Compound (LSC) summary

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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	2.512	182.4	ug/l	9103940	1	8.224	2495700	50.0
Butane, 2-methyl-	3.248	71.5	ug/l	3566680	1	8.224	2495700	50.0
Cyclopropane, e...	3.653	51.0	ug/l	2548060	1	8.224	2495700	50.0
Ethanol	3.824	1312.9	ug/l	65533400	1	8.224	2495700	50.0
2-Butene, 2-met...	4.147	77.7	ug/l	3880220	1	8.224	2495700	50.0
Cyclopentene	5.159	47.5	ug/l	2373100	1	8.224	2495700	50.0
Cyclobutane, me...	5.383	34.4	ug/l	1715410	1	8.224	2495700	50.0
Benzene, 1-ethy...	13.100	60.8	ug/l	3271260	4	13.794	2690500	50.0
Indane	13.994	39.3	ug/l	2113990	4	13.794	2690500	50.0