LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022224\
Data File : VN081133.D
Acq On : 22 Feb 2024 14:24
Operator : JC\MD
Sample : P1540-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1323

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\82N021624W.M
Title : SW846 8260

Signal : TIC: VN081133.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.589	106	108	166	rBV	45926795	223740612	100.00%	79.347%
2	3.783	300	311	324	rBV	883145	2363080	1.06%	0.838%
3	7.224	882	896	925	rBV	3618173	10105949	4.52%	3.584%
4	13.100	1889	1895	1899	rBV	1287316	2530407	1.13%	0.897%
5	13.259	1914	1922	1929	rBV	2586196	4171061	1.86%	1.479%
6	13.341	1929	1936	1943	rVB	2837298	4402330	1.97%	1.561%
7	13.482	1954	1960	1975	rVB	3000588	5401393	2.41%	1.916%
8	13.688	1988	1995	2001	rBV2	1497585	2708798	1.21%	0.961%
9	13.876	2022	2027	2034	rVV	2941212	4638899	2.07%	1.645%
10	13.994	2042	2047	2062	rVV4	1426555	4814302	2.15%	1.707%
11	14.929	2201	2206	2218	rVB4	1321690	3126202	1.40%	1.109%
12	15.053	2218	2227	2234	rBV2	2105672	4952226	2.21%	1.756%
13	15.212	2247	2254	2261	rBV	1976078	3471184	1.55%	1.231%
14	16.170	2412	2417	2427	rVB	1538840	3226209	1.44%	1.144%
15	16.506	2463	2474	2489	rBV	939797	2326242	1.04%	0.825%

Sum of corrected areas: 281978894

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022224\
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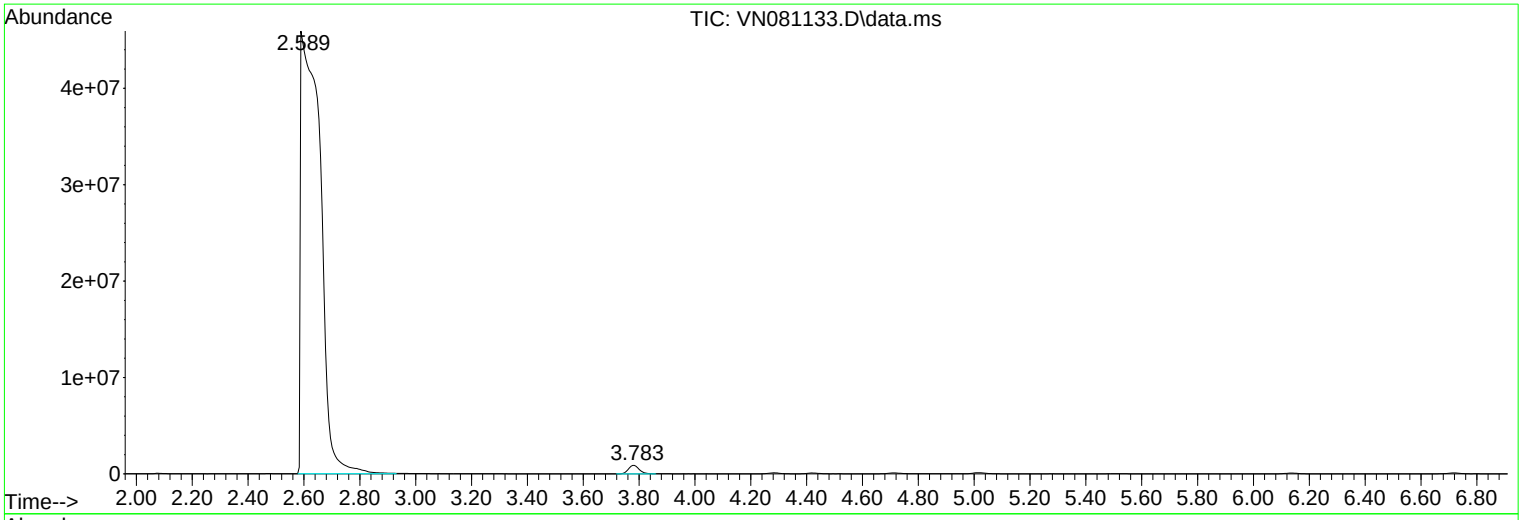
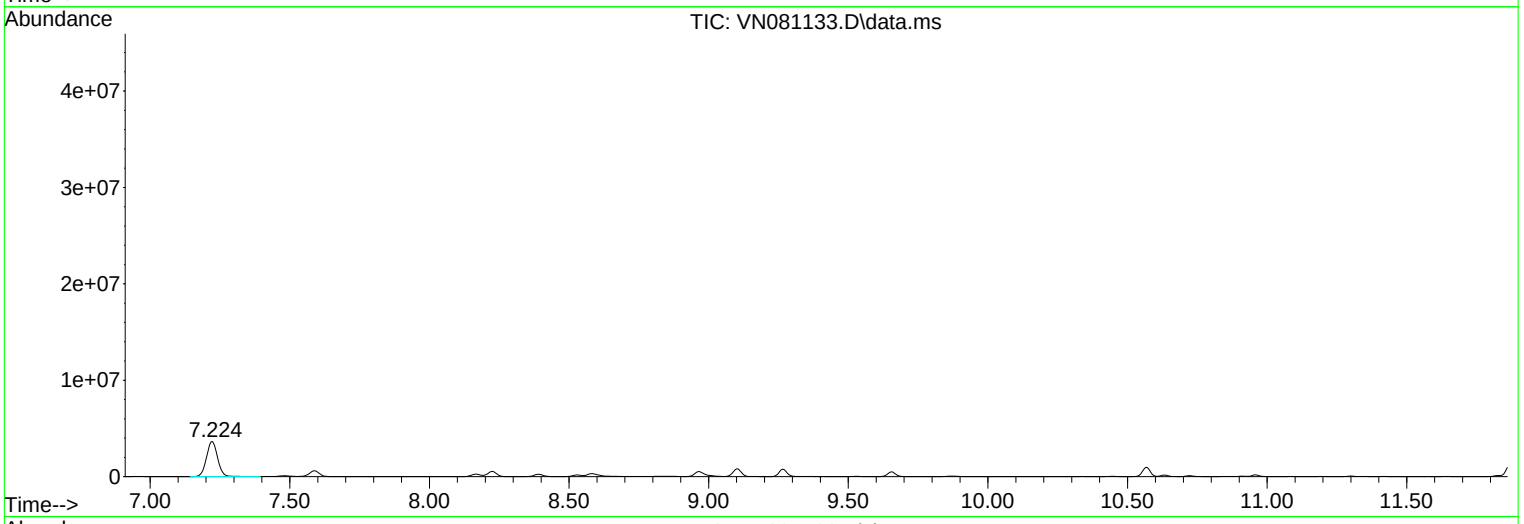
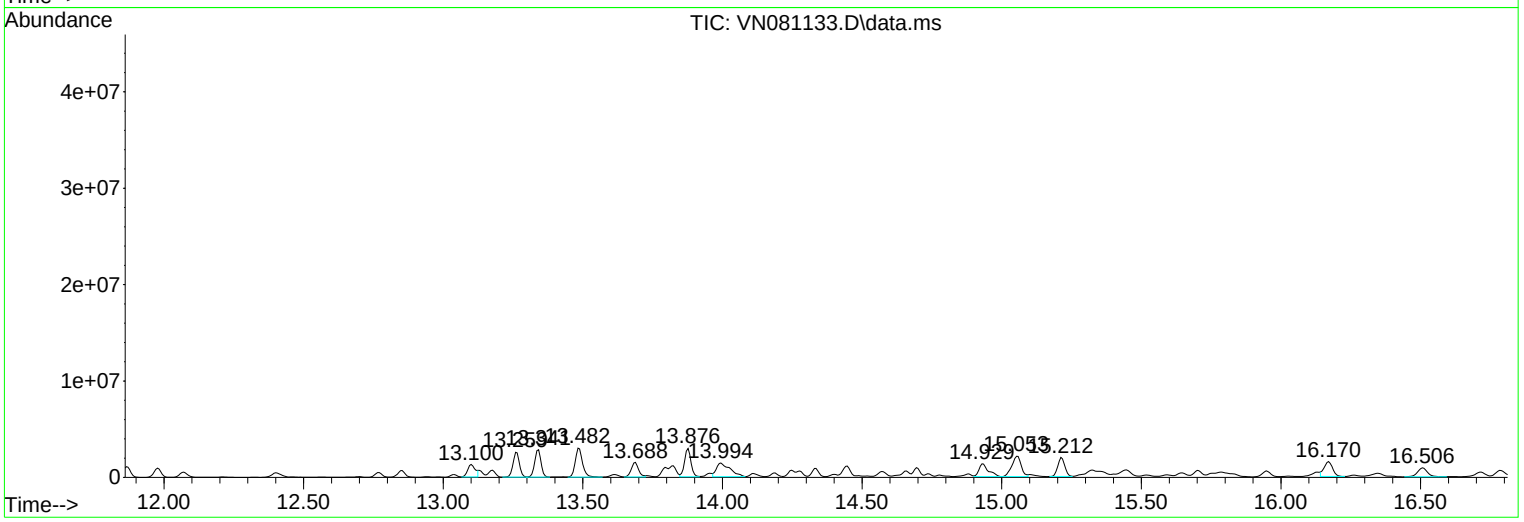
Instrument :
MSVOA_N
ClientSampleId :
AUD-1323

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

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







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Data File : VN081133.D
Acq On : 22 Feb 2024 14:24
Operator : JC\MD
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

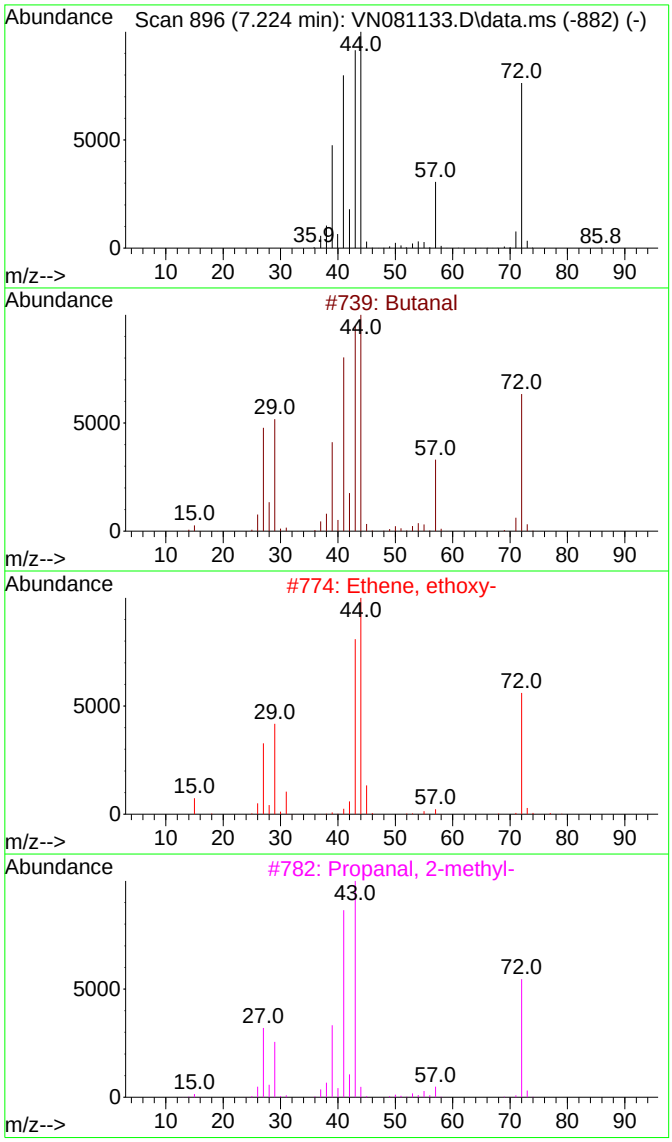
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

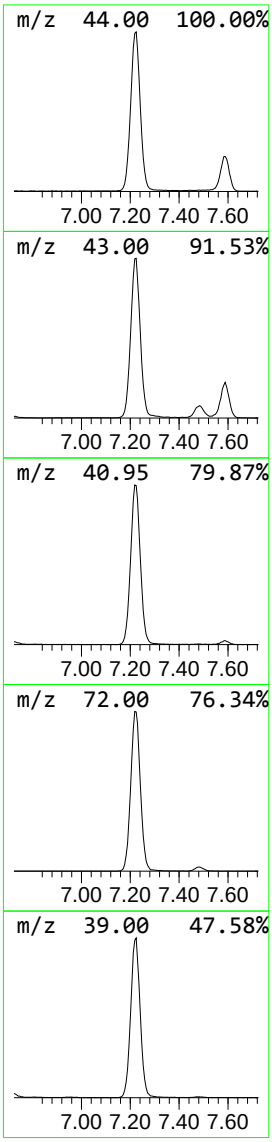
****

Peak Number 2 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	50.00 ug/l	10105900	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	52
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	43
5	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37





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Data File : VN081133.D
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Operator : JC\MD
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Instrument :
MSVOA_N
ClientSampleId :
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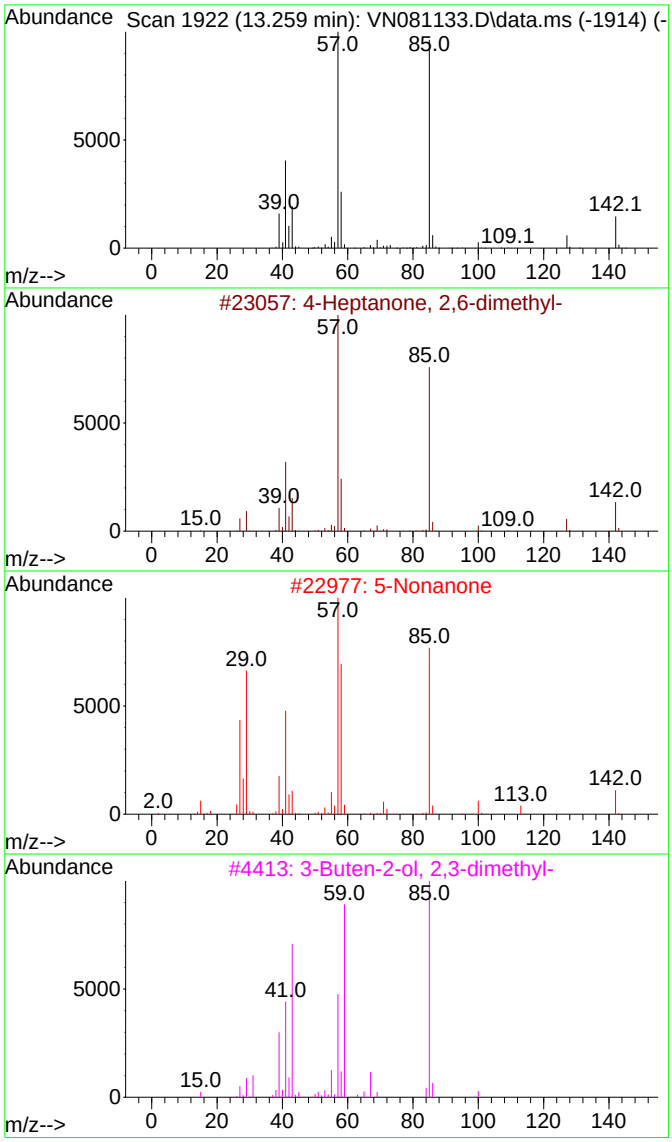
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

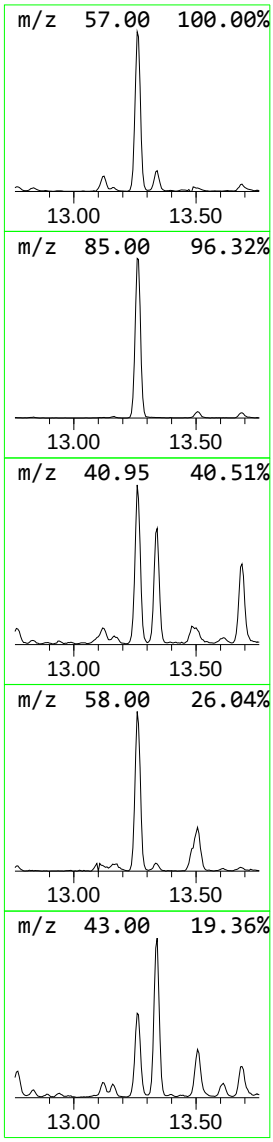
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 4-Heptanone, 2,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.259	44.96 ug/l	4171060	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	94
2	5-Nonanone	142	C9H18O	000502-56-7	64
3	3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	59
4	4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	50
5	2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2	000105-21-5	47





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Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1323

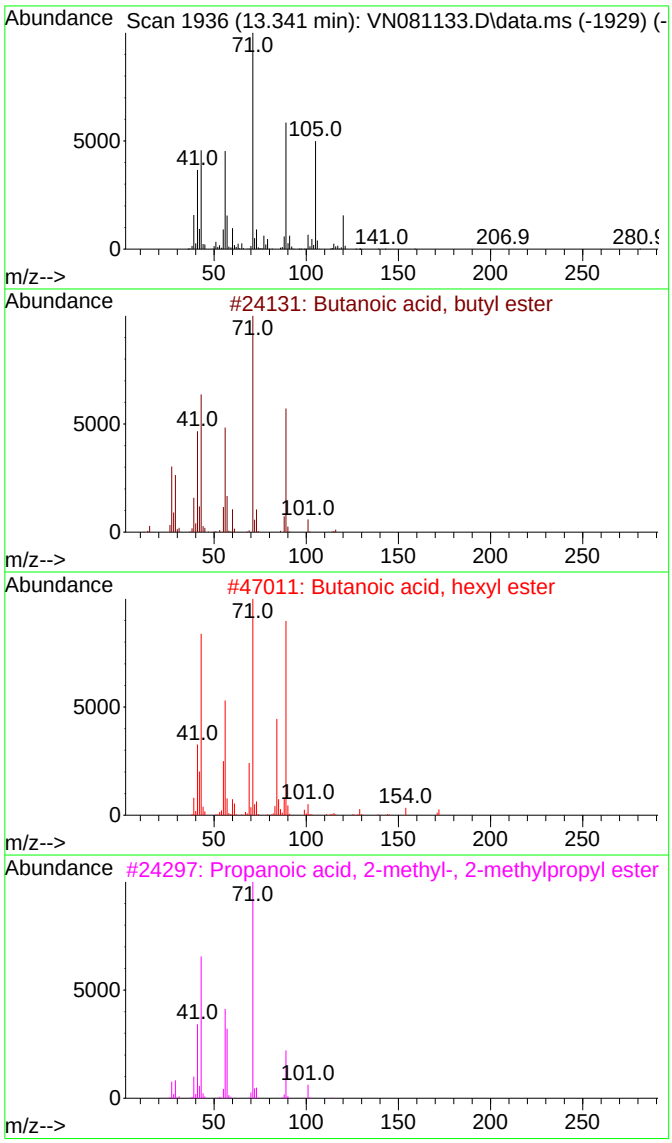
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

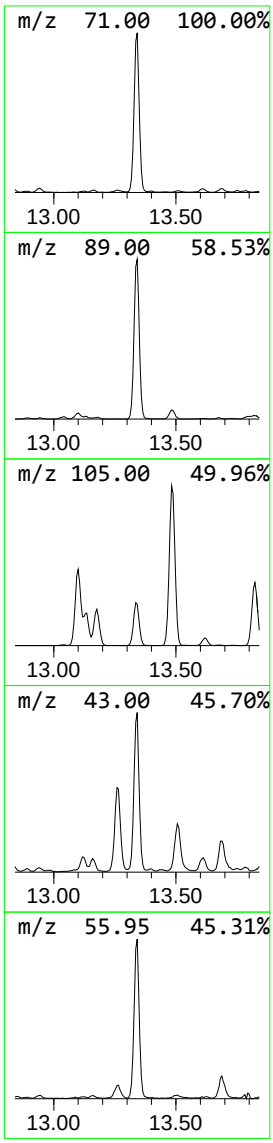
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	47.45 ug/l	4402330	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	80
2	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	56
3	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	53
4	Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	53
5	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	53





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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1323

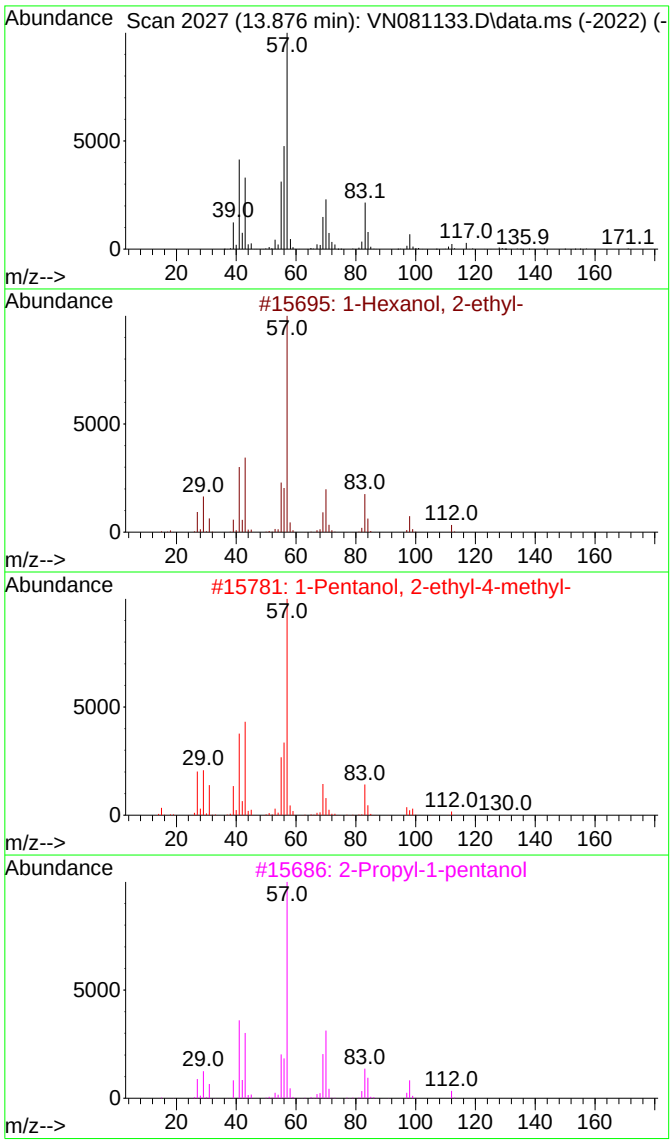
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

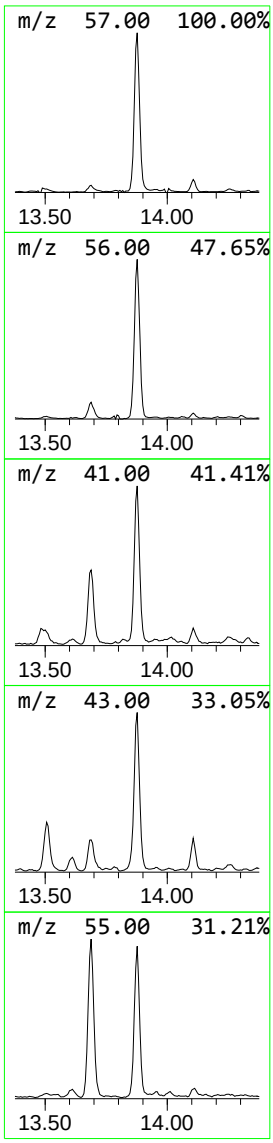
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	50.00 ug/l	4638900	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	49
5	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	43





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Data File : VN081133.D
Acq On : 22 Feb 2024 14:24
Operator : JC\MD
Sample : P1540-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1323

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

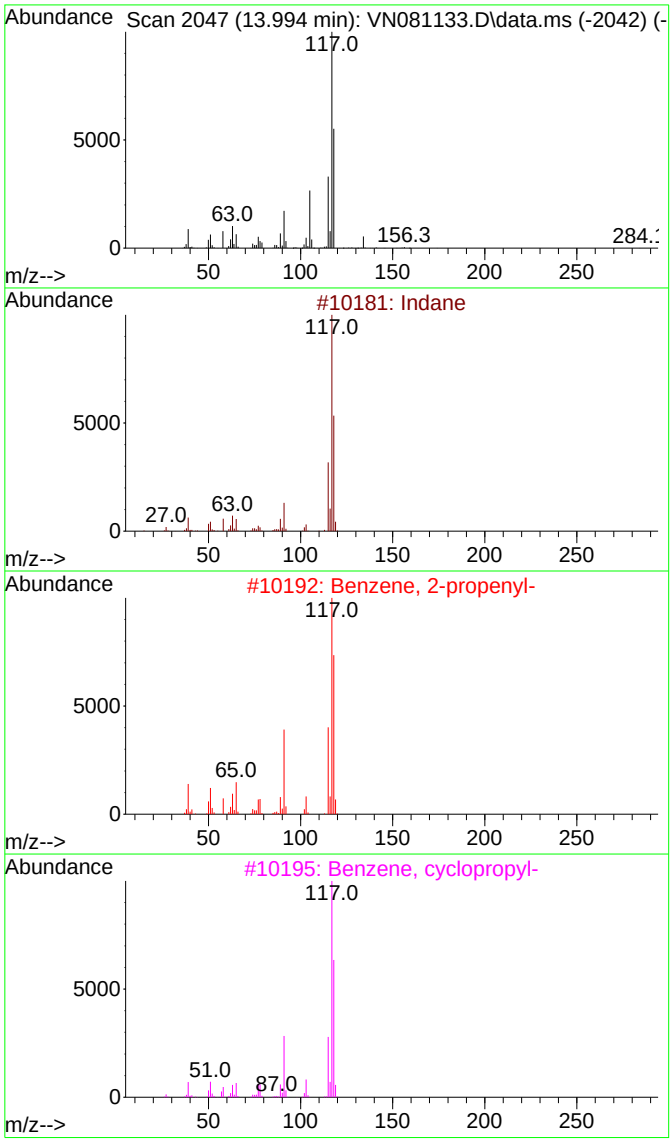
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

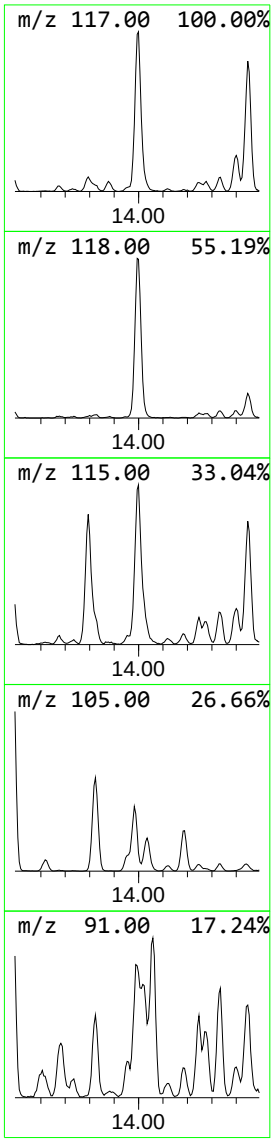
****

Peak Number 6 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	51.89 ug/l	4814300	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	76
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	58
4	Benzeneethanol, .beta.-ethenyl-	148	C10H12O	006052-63-7	47
5	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	47





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Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1323

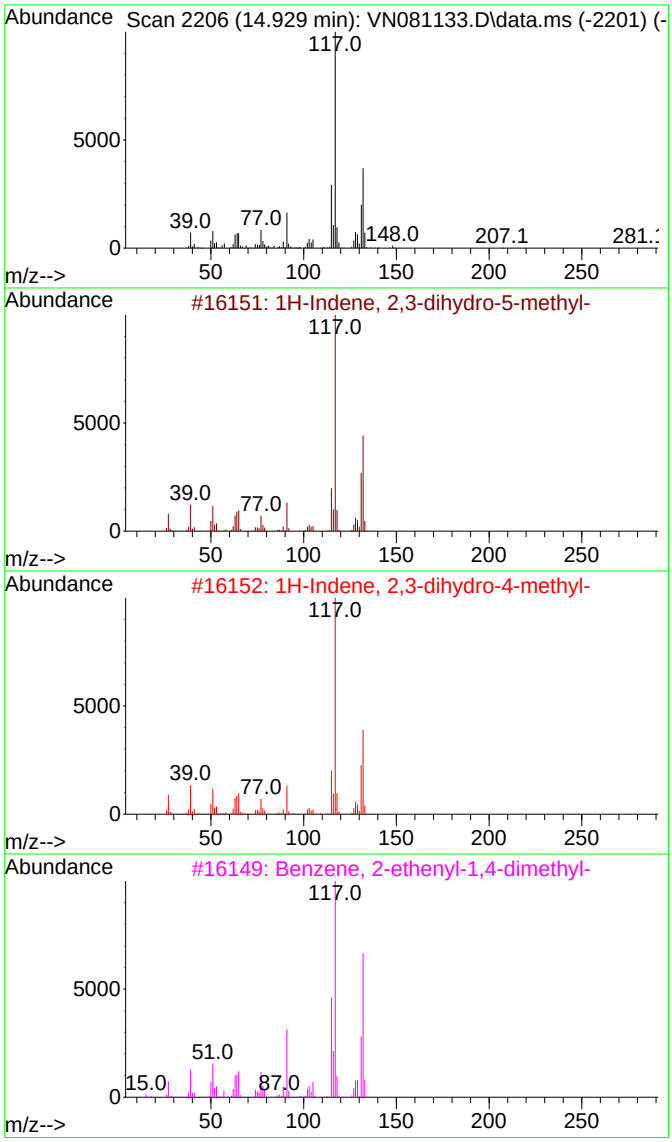
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

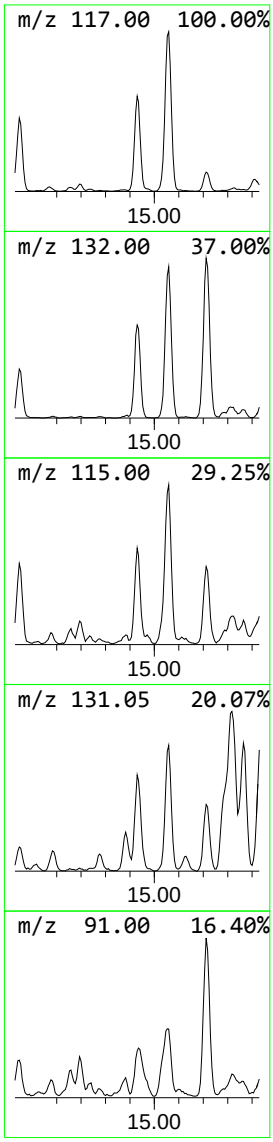
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.929	33.70 ug/l	3126200	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	94
2	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	93
3	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	92
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	91
5	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	90





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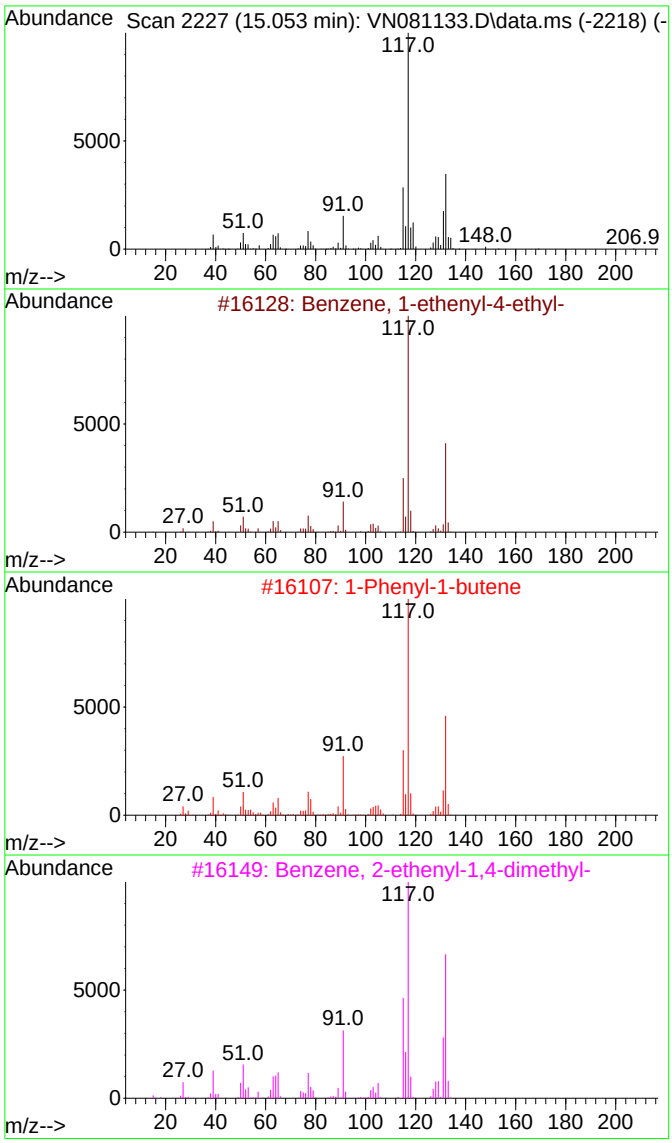
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

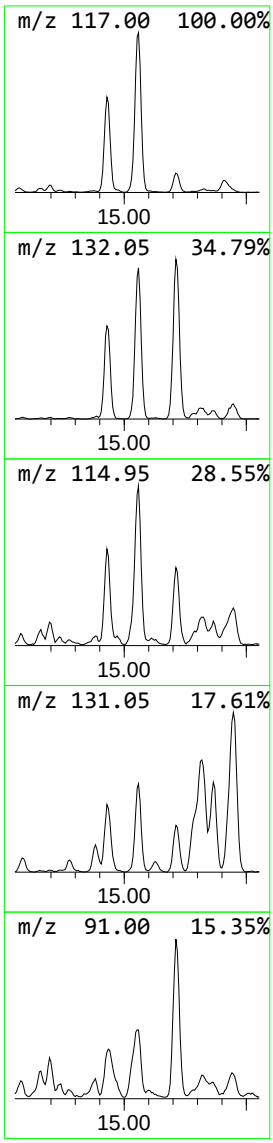
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	53.38 ug/l	4952230	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2	1-Phenyl-1-butene	132	C10H12	000824-90-8	91
3	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
4	Benzene, 2-butenyl-	132	C10H12	001560-06-1	90
5	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	90





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Instrument :
MSVOA_N
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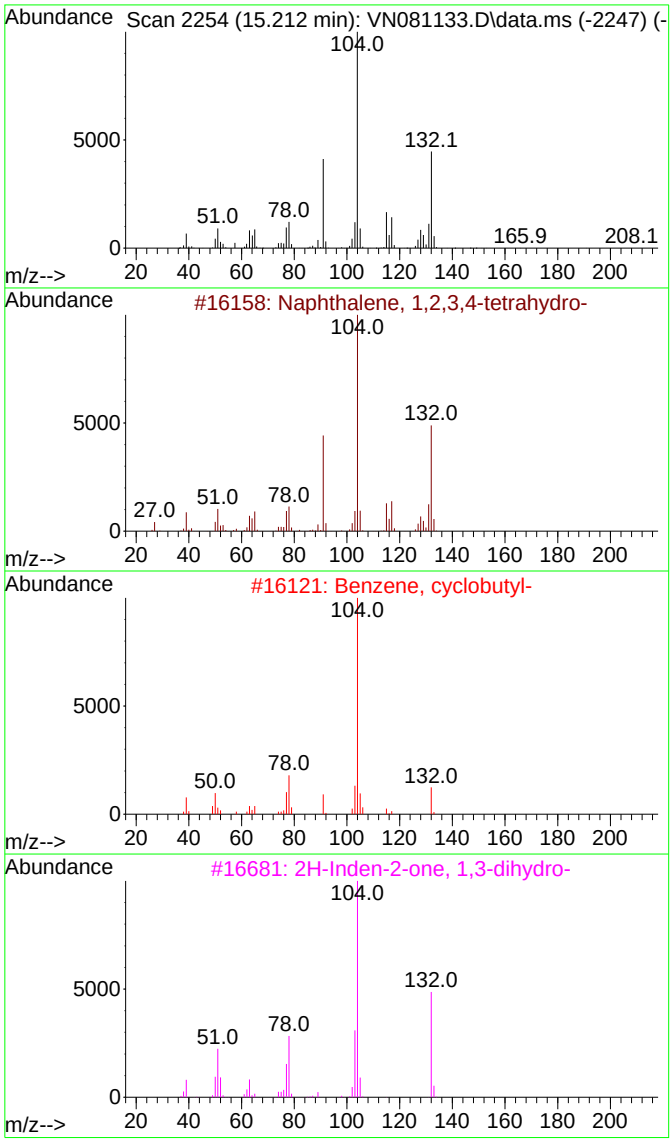
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

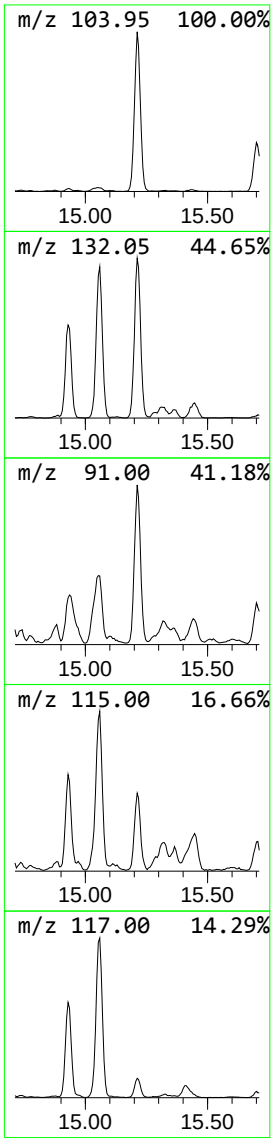
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.212	37.41 ug/l	3471180	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	96
2	Benzene, cyclobutyl-	132	C10H12	004392-30-7	59
3	2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	53
4	Benzene, 1,1'-(1,2-cyclobutanedi...	208	C16H16	020071-09-4	38
5	Indan, epoxide	132	C9H8O	000768-22-9	38





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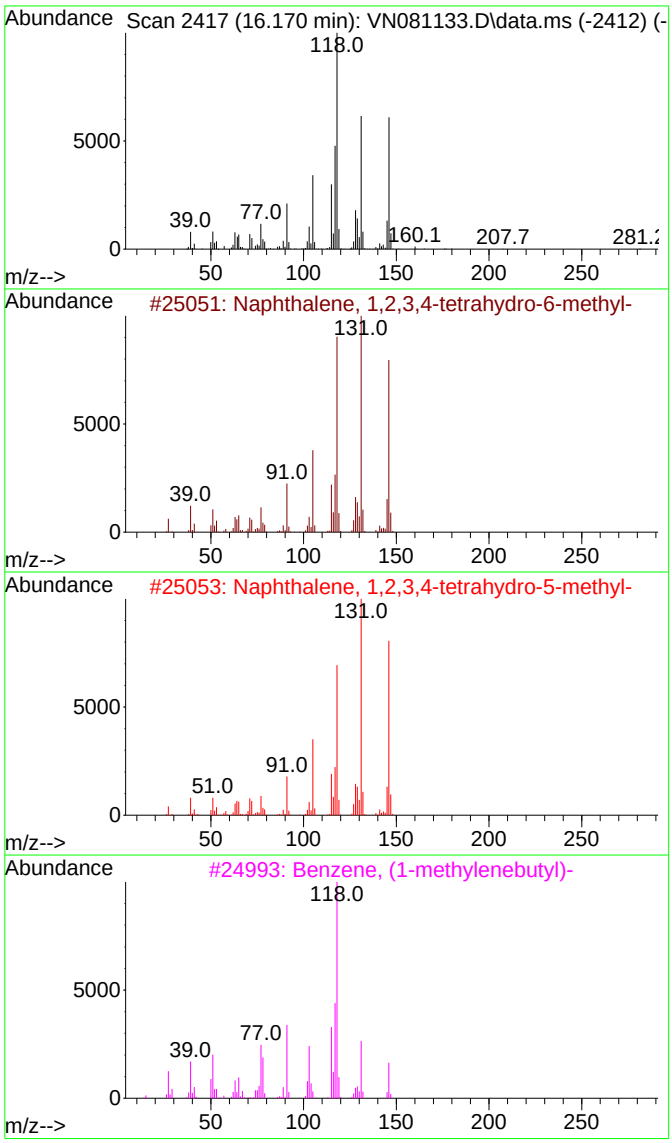
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

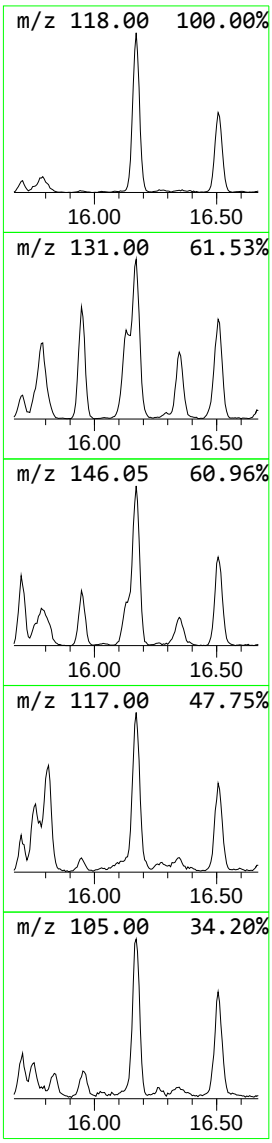
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.170	34.77 ug/l	3226210	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	92
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	92
3	Benzene, (1-methylenebutyl)-	146	C11H14	005676-32-4	83
4	Benzene, (1-ethyl-2-propenyl)-	146	C11H14	019947-22-9	83
5	2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1010189-31-0	58





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butanal	7.224	50.0	ug/l	10105900	1	8.224	10105900	50.0
4-Heptanone, 2,...	13.259	45.0	ug/l	4171060	4	13.794	4638900	50.0
Butanoic acid, ...	13.341	47.5	ug/l	4402330	4	13.794	4638900	50.0
1-Hexanol, 2-et...	13.876	50.0	ug/l	4638900	4	13.794	4638900	50.0
Indane	13.994	51.9	ug/l	4814300	4	13.794	4638900	50.0
1H-Indene, 2,3-...	14.929	33.7	ug/l	3126200	4	13.794	4638900	50.0
Benzene, 1-ethe...	15.053	53.4	ug/l	4952230	4	13.794	4638900	50.0
Naphthalene, 1,...	15.212	37.4	ug/l	3471180	4	13.794	4638900	50.0
Naphthalene, 1,...	16.170	34.8	ug/l	3226210	4	13.794	4638900	50.0