LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065628.D
Acq On : 27 Jan 2021 14:34
Operator : JC/MD
Sample : M1190-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 41110

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\82N012521W.M
Title : SW846 8260

Signal : TIC: VN065628.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.290	158	171	214	rBV	7278235	14581561	100.00%	46.661%
2	3.663	583	598	616	rBV	135867	331221	2.27%	1.060%
3	6.499	1457	1480	1500	rBV2	129325	392056	2.69%	1.255%
4	7.550	1794	1807	1818	rBV2	115712	268952	1.84%	0.861%
5	7.624	1818	1830	1850	rVB	255107	601352	4.12%	1.924%
6	7.991	1920	1944	1967	rBV3	263623	672128	4.61%	2.151%
7	8.547	2102	2117	2141	rBV	391797	820740	5.63%	2.626%
8	9.675	2454	2468	2487	rBV	213706	393340	2.70%	1.259%
9	9.897	2512	2537	2551	rBV2	113861	260267	1.78%	0.833%
10	10.058	2573	2587	2598	rBV	628531	1159719	7.95%	3.711%
11	10.122	2598	2607	2630	rVB	159142	300212	2.06%	0.961%
12	10.772	2794	2809	2822	rBV	638243	1124348	7.71%	3.598%
13	11.376	2984	2997	3022	rVV	667399	1225703	8.41%	3.922%
14	11.515	3022	3040	3052	rVV	1597112	2669221	18.31%	8.542%
15	11.589	3053	3063	3079	rVB	160764	312708	2.14%	1.001%
16	11.929	3157	3169	3176	rBV3	130882	278934	1.91%	0.893%
17	11.974	3176	3183	3191	rVB2	100626	177794	1.22%	0.569%
18	12.373	3290	3307	3319	rVB	398487	698812	4.79%	2.236%
19	12.563	3355	3366	3378	rVB	177766	294275	2.02%	0.942%
20	12.884	3454	3466	3479	rBV2	308373	498455	3.42%	1.595%
21	13.074	3517	3525	3534	rVB	173732	272173	1.87%	0.871%
22	13.222	3563	3571	3584	rVB3	146671	251785	1.73%	0.806%
23	13.312	3588	3599	3616	rBV	483789	829452	5.69%	2.654%
24	13.418	3621	3632	3651	rBV	1115688	1800527	12.35%	5.762%
25	13.691	3706	3717	3733	rBV	258080	448036	3.07%	1.434%
26	15.100	4138	4155	4164	rBV	131011	282782	1.94%	0.905%
27	15.167	4164	4176	4196	rVB3	133512	303403	2.08%	0.971%

Sum of corrected areas: 31249956

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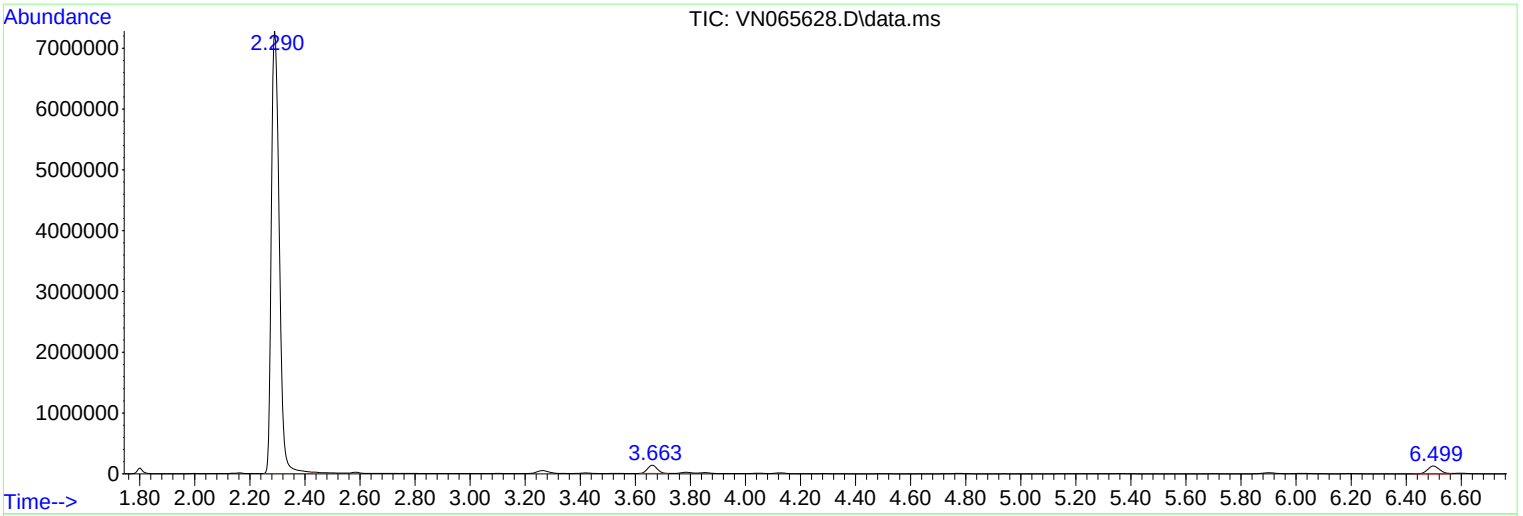
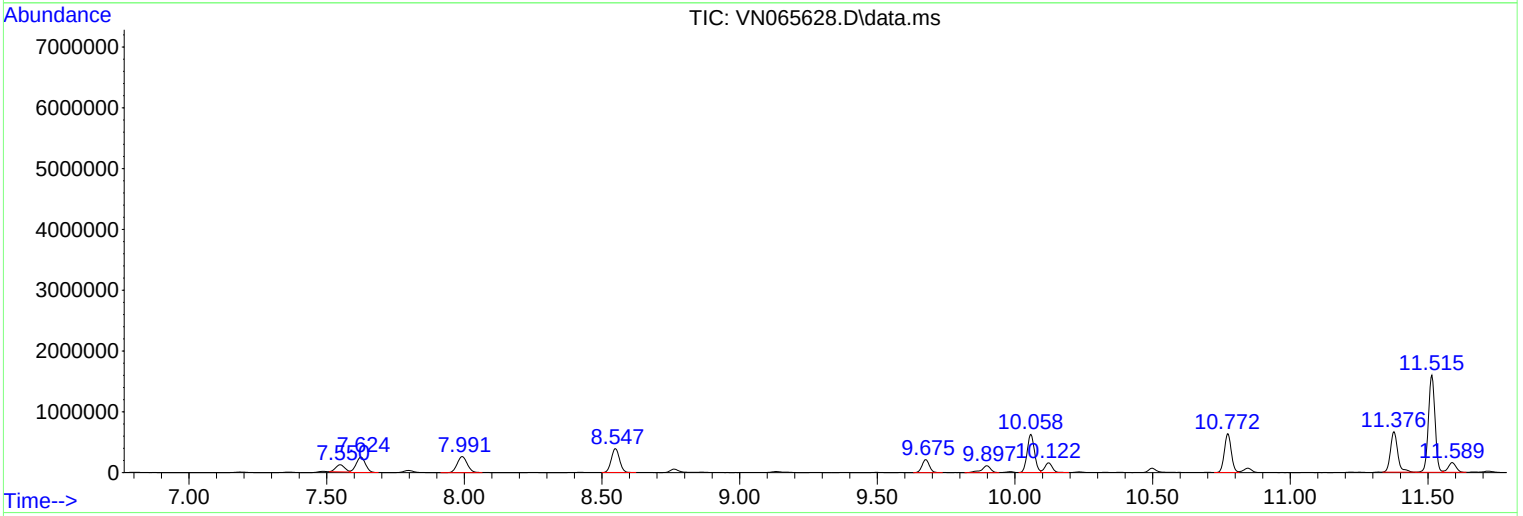
ALS Vial : 11 Sample Multiplier: 1

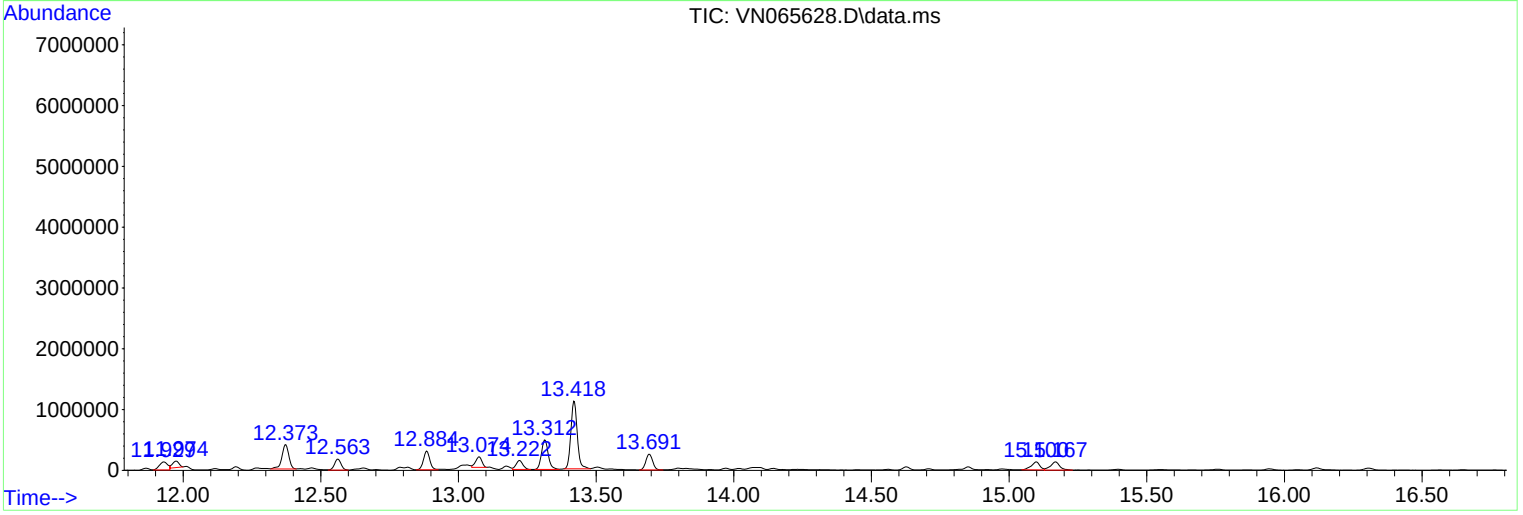
Instrument :
MSVOA_N
ClientSampleId :
41110

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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







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Quant Title : SW846 8260

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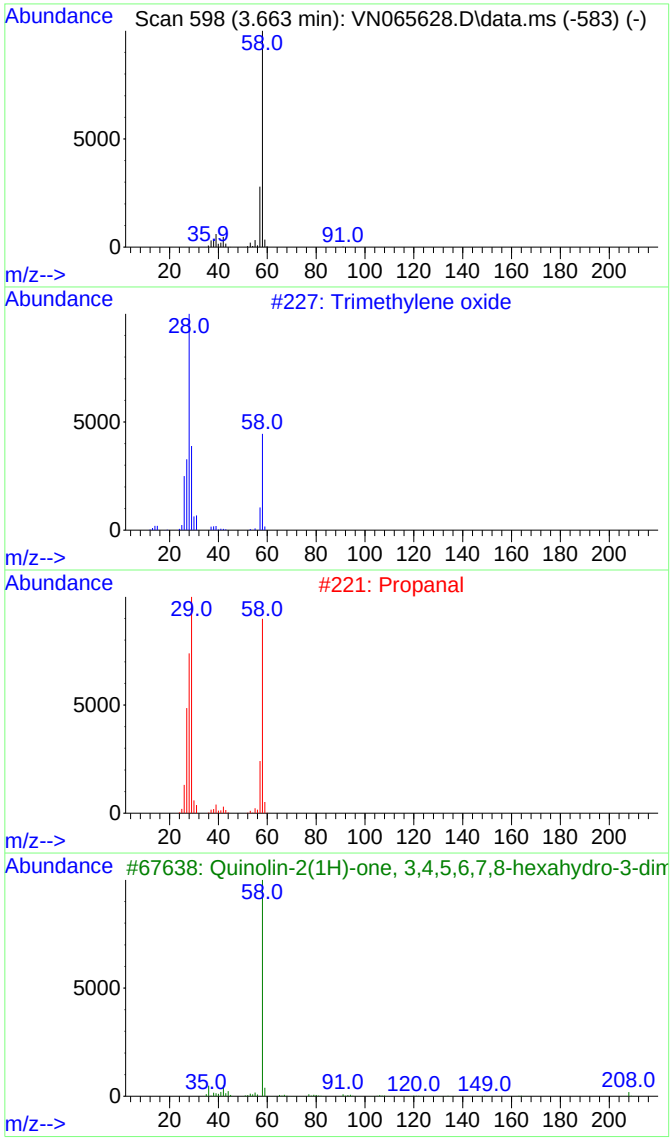
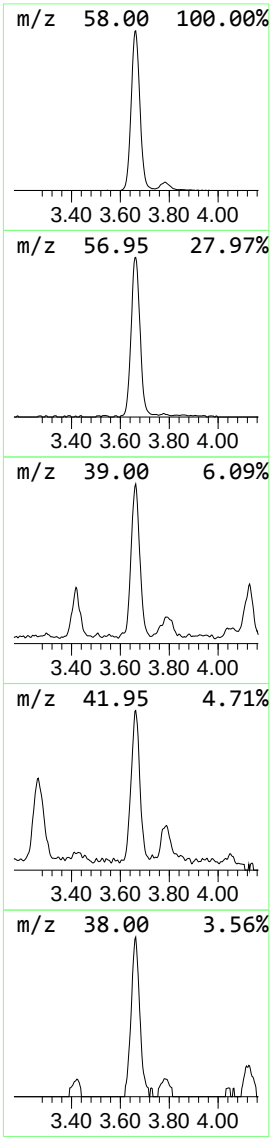
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Trimethylene oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.663	27.54 ug/l	331221	Pentafluorobenzene	7.624

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trimethylene oxide	58	C3H6O	000503-30-0	64
2	Propanal	58	C3H6O	000123-38-6	40
3	Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
4	Borane, compd. with dimethylamin...	59	C2H10BN	000074-94-2	7
5	Propylene oxide	58	C3H6O	000075-56-9	5





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Data File : VN065628.D
Acq On : 27 Jan 2021 14:34
Operator : JC/MD
Sample : M1190-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 41110

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

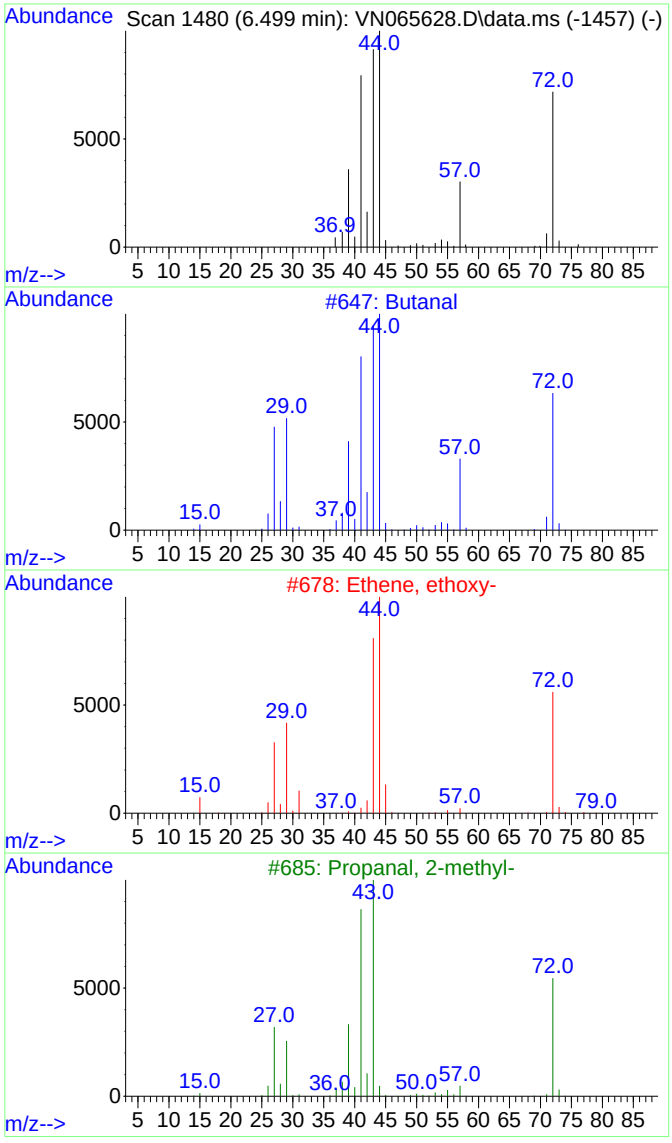
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

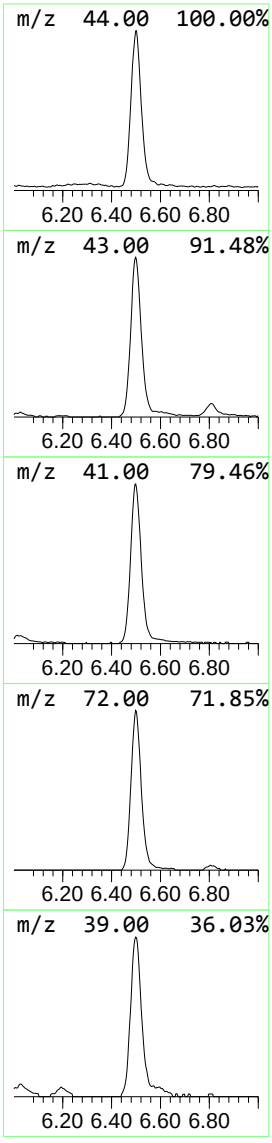
****

Peak Number 3 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.499	32.60 ug/l	392056	Pentafluorobenzene	7.624

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	59
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	46
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	27
5	Isobutylene epoxide	72	C4H8O	000558-30-5	27





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Data File : VN065628.D
Acq On : 27 Jan 2021 14:34
Operator : JC/MD
Sample : M1190-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 41110

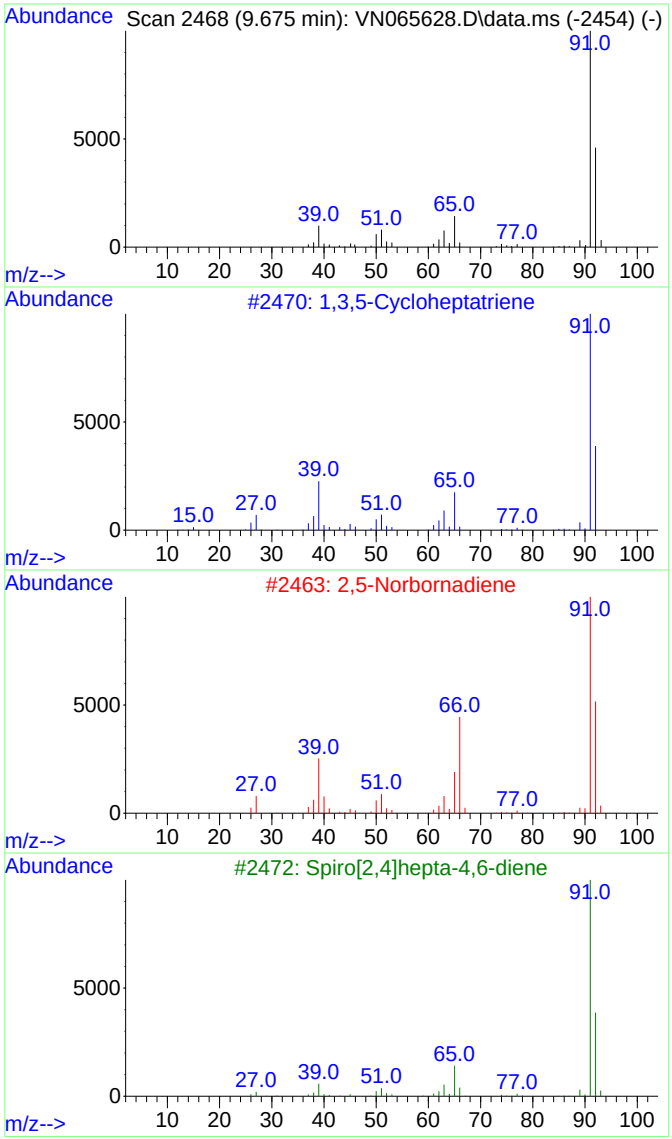
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

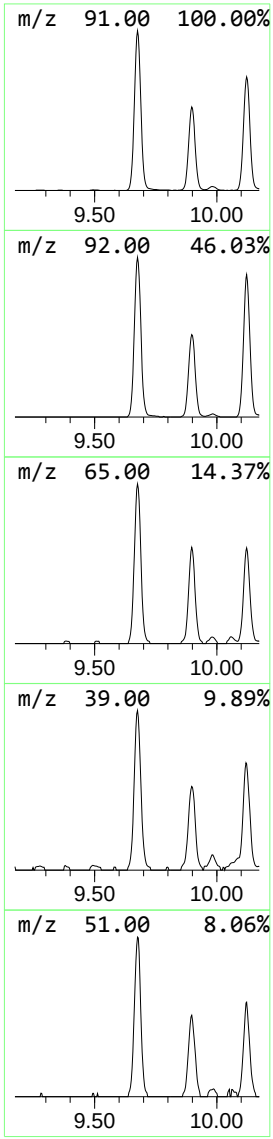
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1,3,5-Cycloheptatriene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.675	23.96 ug/l	393340	1,4-Difluorobenzene	8.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	91
2	2,5-Norbornadiene	92	C7H8	000121-46-0	91
3	Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	91
4	Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	91
5	Toluene	92	C7H8	000108-88-3	91





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Operator : JC/MD
Sample : M1190-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 41110

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

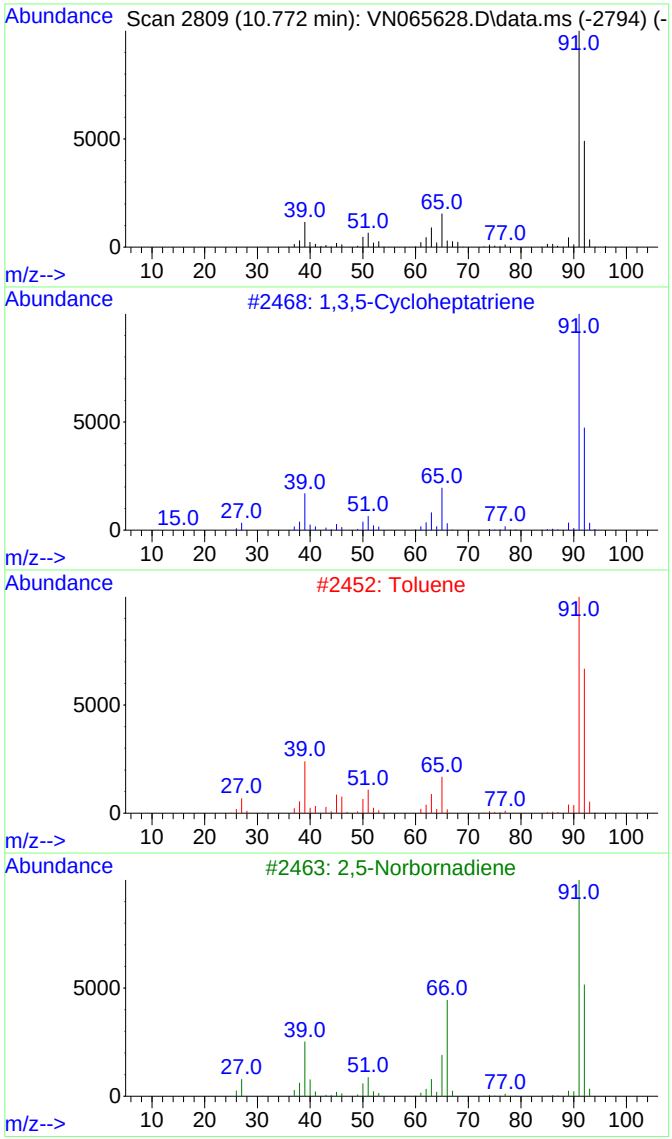
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

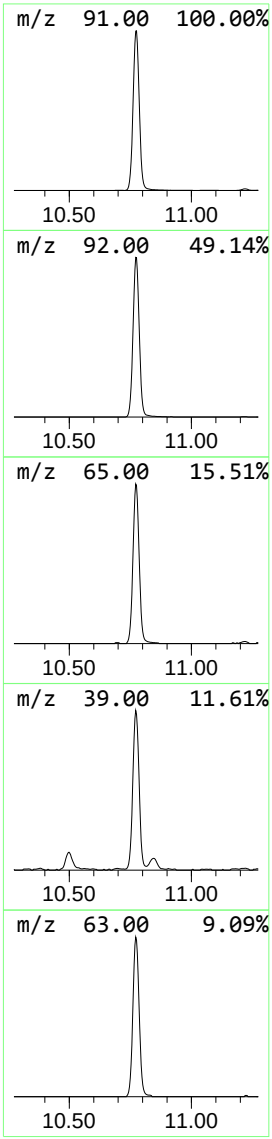
****

Peak Number 5 2,5-Norbornadiene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.772	45.87 ug/l	1124350	Chlorobenzene-d5	11.376

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	94
2	Toluene	92	C7H8	000108-88-3	91
3	2,5-Norbornadiene	92	C7H8	000121-46-0	90
4	Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	90
5	Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	90





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Operator : JC/MD
Sample : M1190-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 41110

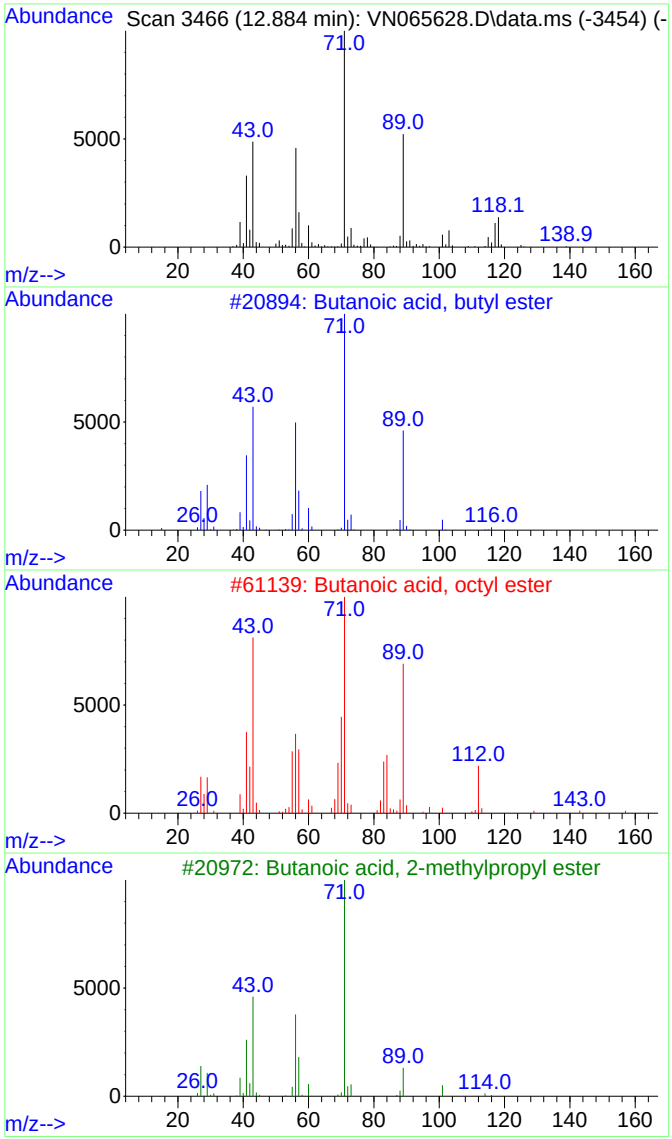
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

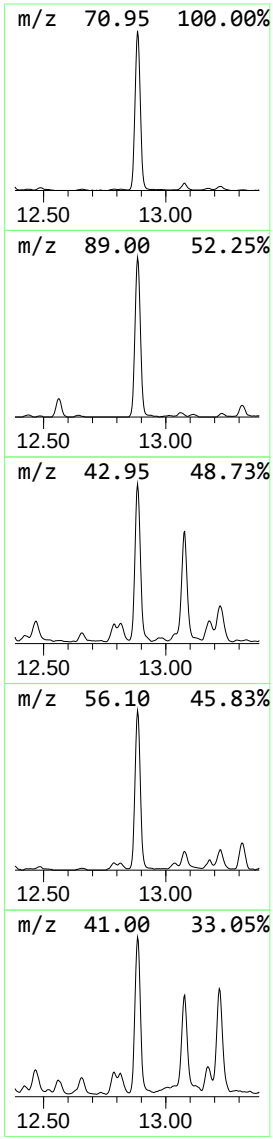
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Butanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.884	30.05 ug/l	498455	1,4-Dichlorobenzene-d4	13.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	80
2	Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	72
3	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	53
4	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	50
5	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	45





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Instrument : MSVOA_N
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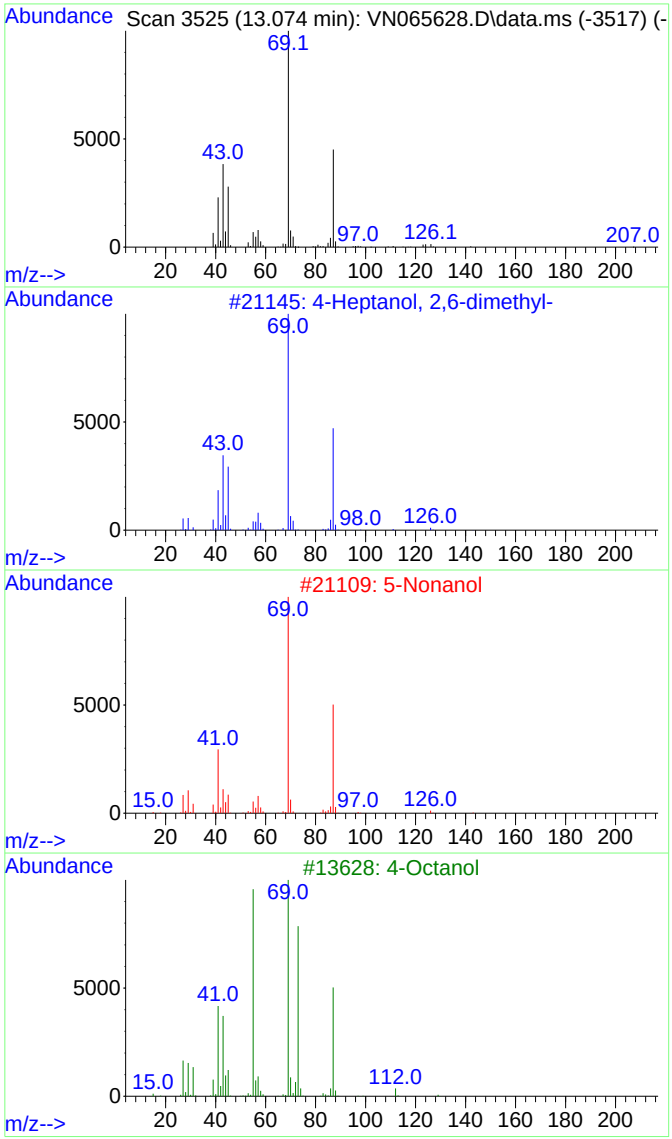
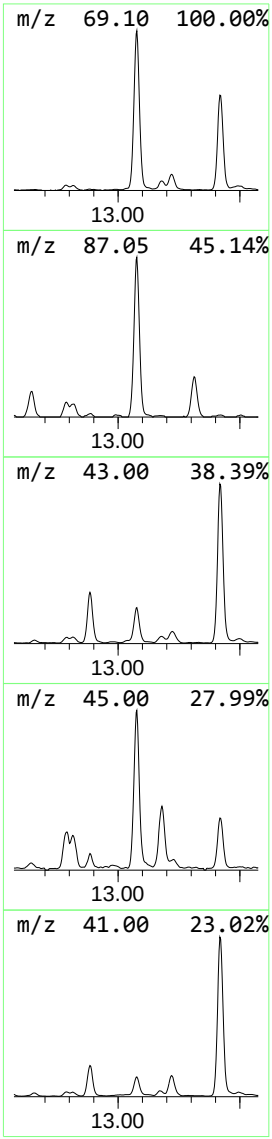
****
Peak Number 7 4-Heptanol, 2,6-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.074	16.41 ug/l	272173	1,4-Dichlorobenzene-d4	13.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	90
2	5-Nonanol	144	C9H20O	000623-93-8	72
3	4-Octanol	130	C8H18O	000589-62-8	72
4	Cyclopropanecarboxylic acid, pro...	128	C7H12O2	060128-01-0	64
5	2-Hydroxyethyl methacrylate	130	C6H10O3	000868-77-9	64





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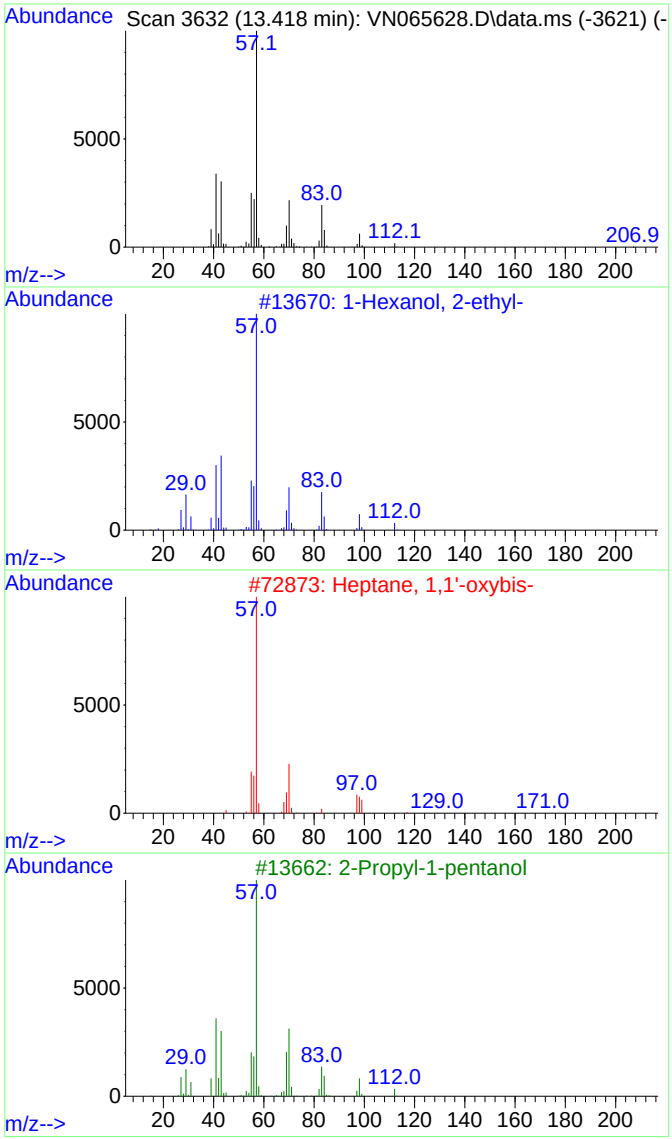
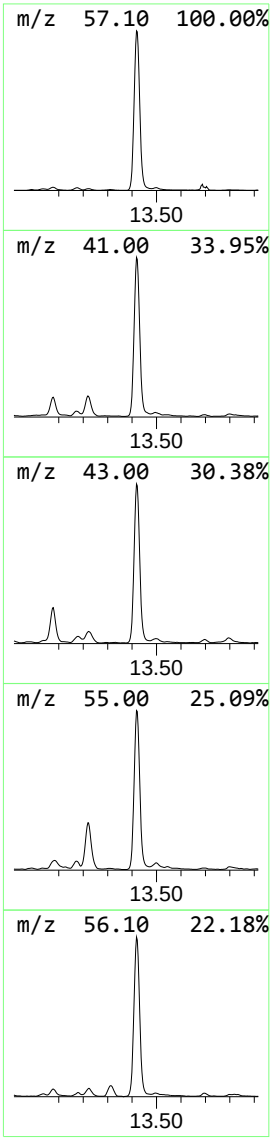
****
Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.418	108.54 ug/l	1800530	1,4-Dichlorobenzene-d4	13.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4	Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	47
5	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47





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Quant Title : SW846 8260

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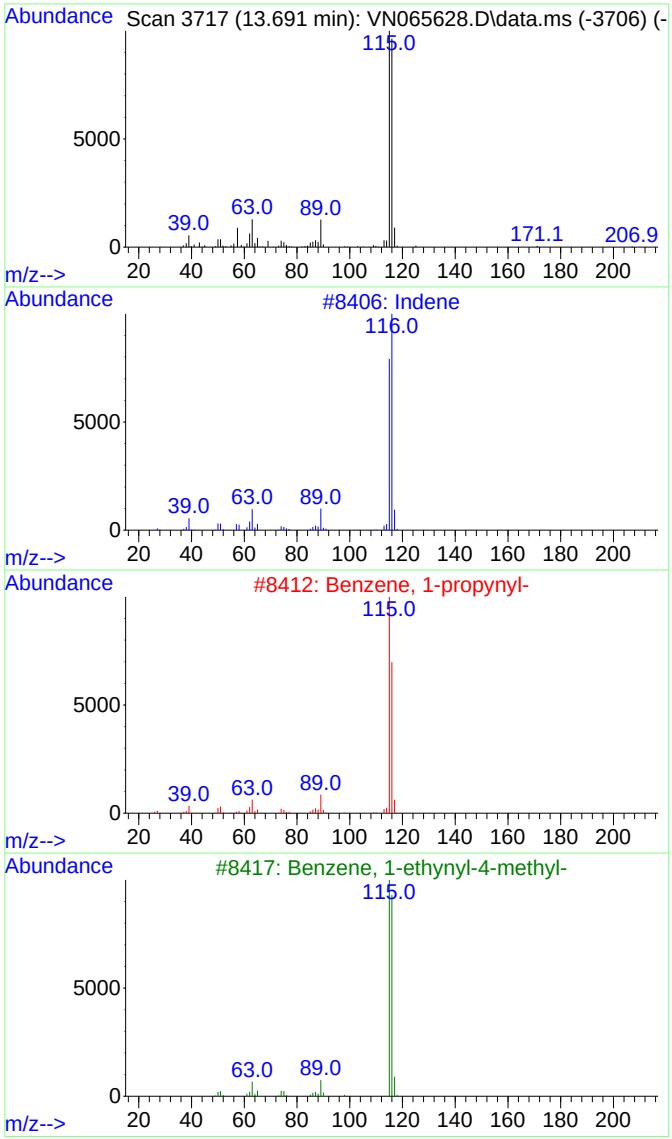
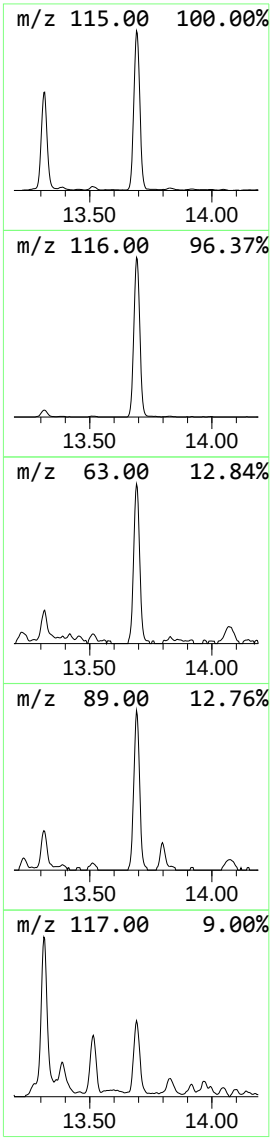
****
Peak Number 9 Indene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.691	27.01 ug/l	448036	1,4-Dichlorobenzene-d4	13.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	97
2	Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
3	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
4	3-Methylphenylacetylene	116	C9H8	000766-82-5	91
5	2-Methylphenylacetylene	116	C9H8	000766-47-2	91





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ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 41110

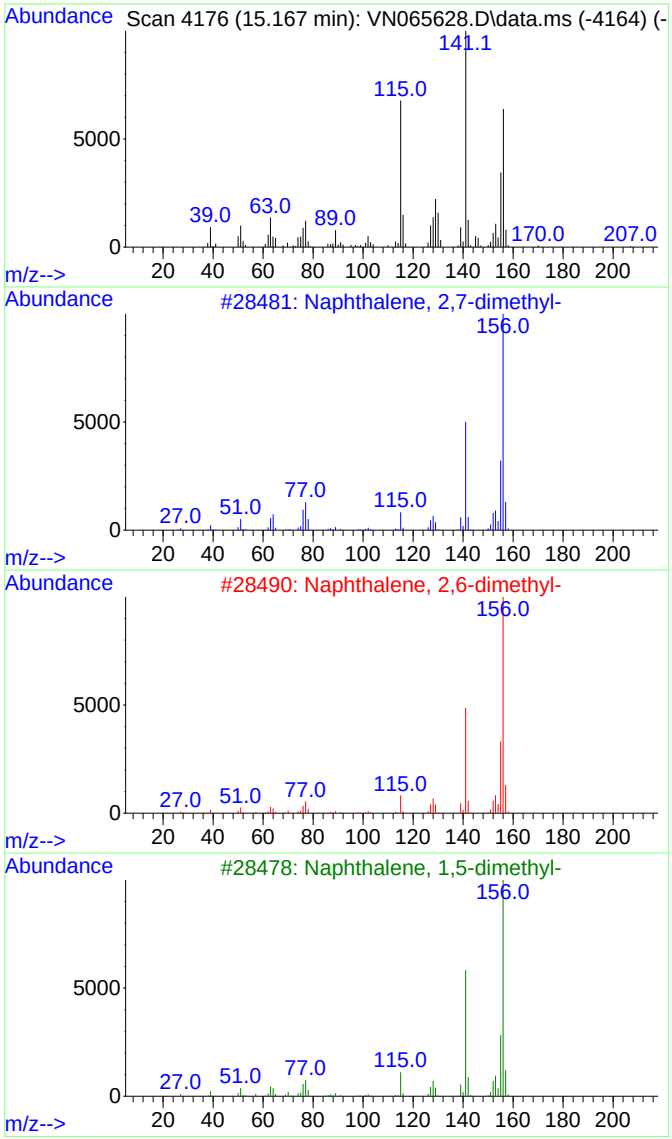
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

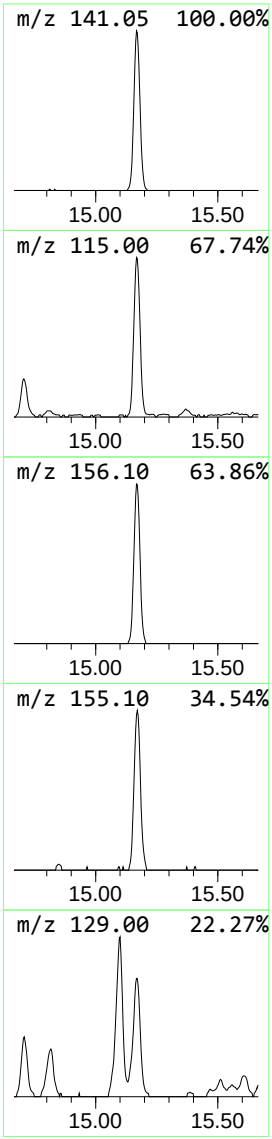
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 2,7-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.167	18.29 ug/l	303403	1,4-Dichlorobenzene-d4	13.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	94
2	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	93
3	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	89
4	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	86
5	Naphthalene, 1-ethyl-	156	C12H12	001127-76-0	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065628.D
Acq On : 27 Jan 2021 14:34
Operator : JC/MD
Sample : M1190-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 41110

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.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
Trimethylene oxide	3.663	27.5	ug/l	331221	1	7.624	601352	50.0
Butanal	6.499	32.6	ug/l	392056	1	7.624	601352	50.0
1,3,5-Cyclohept...	9.675	24.0	ug/l	393340	2	8.550	820740	50.0
2,5-Norbornadiene	10.772	45.9	ug/l	1124350	3	11.376	1225700	50.0
Butanoic acid, ...	12.884	30.1	ug/l	498455	4	13.315	829452	50.0
4-Heptanol, 2,6...	13.074	16.4	ug/l	272173	4	13.315	829452	50.0
1-Hexanol, 2-et...	13.418	108.5	ug/l	1800530	4	13.315	829452	50.0
Indene	13.691	27.0	ug/l	448036	4	13.315	829452	50.0
Naphthalene, 2,...	15.167	18.3	ug/l	303403	4	13.315	829452	50.0