LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067290.D
Acq On : 11 Jun 2021 15:54
Operator : JC/MD
Sample : M2674-06 10X
Misc : 4.91g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TMR-DS-06-060921

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\82N061021W.M
Title : SW846 8260

Signal : TIC: VN067290.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.021	2226	2249	2260	rBV2	335587	800848	6.05%	0.560%
2	8.086	2261	2273	2295	rVB2	630834	1430363	10.81%	0.999%
3	8.440	2384	2405	2435	rBV	420106	1014414	7.67%	0.709%
4	8.968	2584	2602	2631	rBV2	909299	1953961	14.77%	1.365%
5	9.271	2702	2715	2736	rVB2	114348	224289	1.69%	0.157%
6	10.443	3131	3152	3164	rBV	1431134	2714607	20.51%	1.897%
7	10.507	3165	3176	3203	rVB	995783	2017088	15.24%	1.409%
8	10.625	3210	3220	3237	rVB3	107137	206785	1.56%	0.144%
9	10.816	3277	3291	3303	rBV	368330	641077	4.84%	0.448%
10	11.060	3370	3382	3405	rVB6	148861	315997	2.39%	0.221%
11	11.521	3544	3554	3573	rVB2	149320	255999	1.93%	0.179%
12	11.747	3623	3638	3660	rVB	1340392	2420834	18.29%	1.692%
13	11.846	3661	3675	3688	rBV	1287244	2210067	16.70%	1.544%
14	11.907	3689	3698	3700	rVV2	222414	282626	2.14%	0.197%
15	11.950	3701	3714	3740	rVB2	3886545	7683612	58.06%	5.369%
16	12.176	3790	3798	3815	rVB	261987	464936	3.51%	0.325%
17	12.283	3824	3838	3855	rVV	2050104	3617421	27.34%	2.528%
18	12.353	3857	3864	3885	rVB4	104695	213285	1.61%	0.149%
19	12.484	3903	3913	3935	rBV5	269477	560985	4.24%	0.392%
20	12.578	3938	3948	3959	rVV2	227729	412106	3.11%	0.288%
21	12.634	3962	3969	3983	rVB8	120879	230263	1.74%	0.161%
22	12.734	3986	4006	4028	rVB2	1235701	2411200	18.22%	1.685%
23	12.873	4043	4058	4066	rBV6	308774	678841	5.13%	0.474%
24	12.921	4066	4076	4088	rBV	909281	1405185	10.62%	0.982%
25	12.986	4088	4100	4106	rBV	2087068	3508906	26.52%	2.452%
26	13.222	4173	4188	4204	rVB	1398498	2602600	19.67%	1.819%
27	13.369	4231	4243	4254	rVV	3321294	5228294	39.51%	3.653%
28	13.417	4255	4261	4273	rVB2	420204	629889	4.76%	0.440%
29	13.592	4317	4326	4345	rVB2	1465526	2844208	21.49%	1.987%
30	13.678	4346	4358	4361	rBV	1375859	2007959	15.17%	1.403%
31	13.873	4409	4431	4441	rBV6	1949829	4848200	36.64%	3.388%
32	13.997	4471	4477	4488	rVB3	712807	1003591	7.58%	0.701%
33	14.058	4489	4500	4516	rVB2	1551574	3012845	22.77%	2.105%
34	14.133	4518	4528	4532	rBV2	601288	902773	6.82%	0.631%
35	14.217	4550	4559	4570	rVB2	1025858	1594410	12.05%	1.114%
36	14.329	4591	4601	4625	rVB4	1071965	2583190	19.52%	1.805%

LSC Area Percent Report

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Operator : JC/MD
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ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TMR-DS-06-060921

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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Title : SW846 8260

37	14.442	4632	4643	4658	rVB4	737835	1645804	12.44%	1.150%
38	14.514	4659	4670	4680	rBV	1764478	3125658	23.62%	2.184%
39	14.635	4690	4715	4725	rBV2	5114671	13233477	100.00%	9.247%
40	14.817	4770	4783	4807	rVB7	1992089	5730282	43.30%	4.004%
41	14.933	4809	4826	4840	rVV4	1693167	4728412	35.73%	3.304%
42	14.997	4841	4850	4869	rVB2	2636574	4660877	35.22%	3.257%
43	15.086	4871	4883	4901	rVB2	2255774	4252283	32.13%	2.971%
44	15.453	4999	5020	5029	rBV	3708921	9599566	72.54%	6.708%
45	15.587	5058	5070	5084	rBV	6528069	11572493	87.45%	8.086%
46	15.673	5094	5102	5112	rBV	1502646	2168992	16.39%	1.516%
47	16.443	5380	5389	5404	rVB2	1248433	2497996	18.88%	1.745%
48	16.520	5407	5418	5432	rVB	1455643	3077326	23.25%	2.150%
49	16.614	5441	5453	5473	rVB2	3856455	9352756	70.67%	6.535%
50	16.759	5496	5507	5518	rBV4	1189626	2533427	19.14%	1.770%

Sum of corrected areas: 143113003

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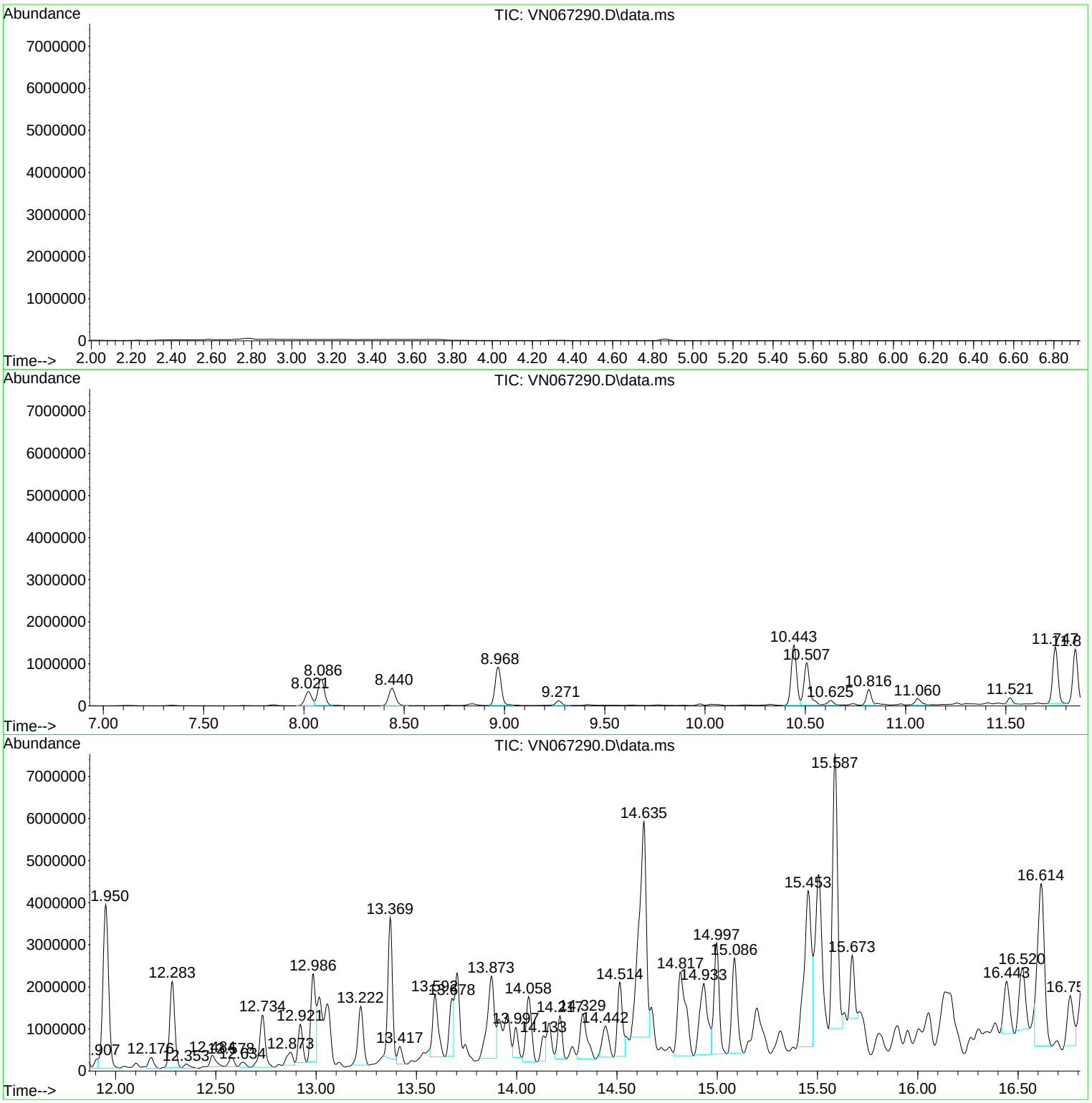
Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-06-060921

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067290.D
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Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-06-060921

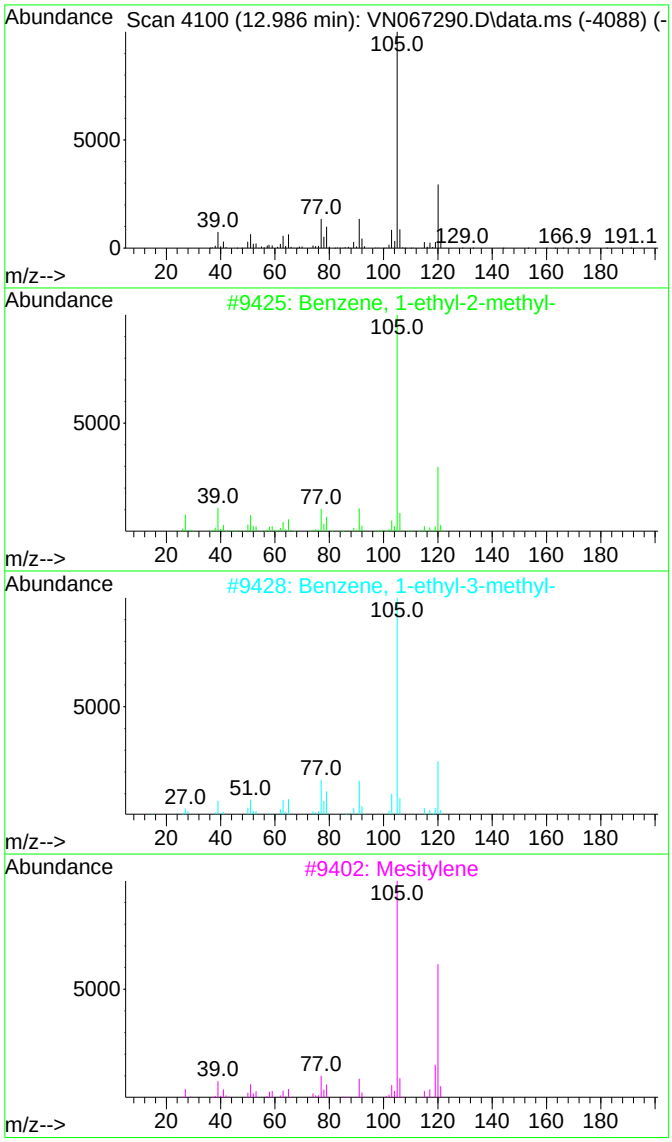
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

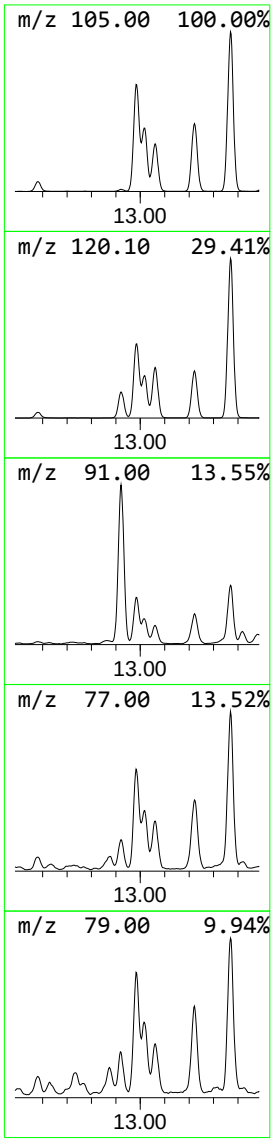
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Benzene, 1-ethyl-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.986	87.37 ug/l	3508910	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





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Data File : VN067290.D
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Operator : JC/MD
Sample : M2674-06 10X
Misc : 4.91g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-06-060921

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

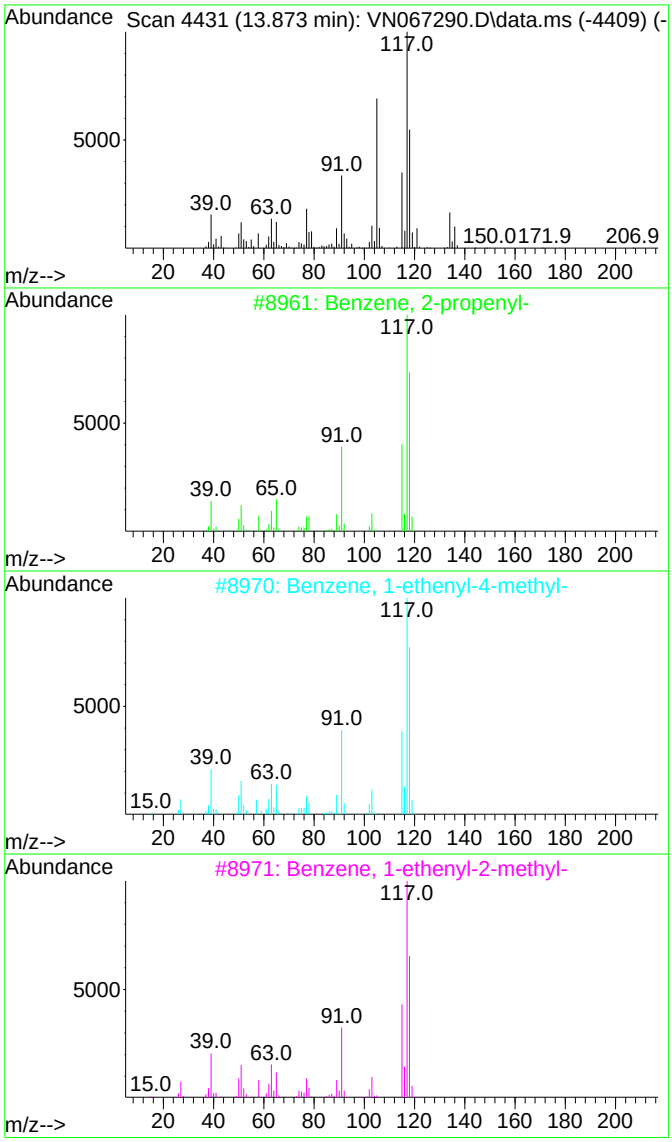
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

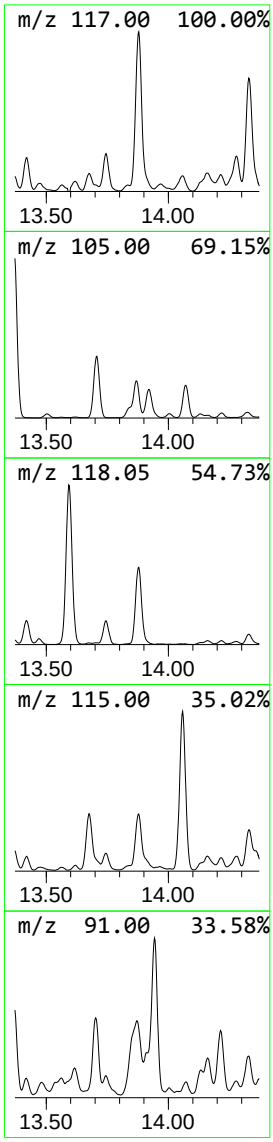
****

Peak Number 2 Benzene, 2-propenyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.873	120.72 ug/l	4848200	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-propenyl-	118	C9H10	000300-57-2	93
2	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	89
3	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	86
4	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	86
5	Benzene, cyclopropyl-	118	C9H10	000873-49-4	70





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067290.D
Acq On : 11 Jun 2021 15:54
Operator : JC/MD
Sample : M2674-06 10X
Misc : 4.91g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-06-060921

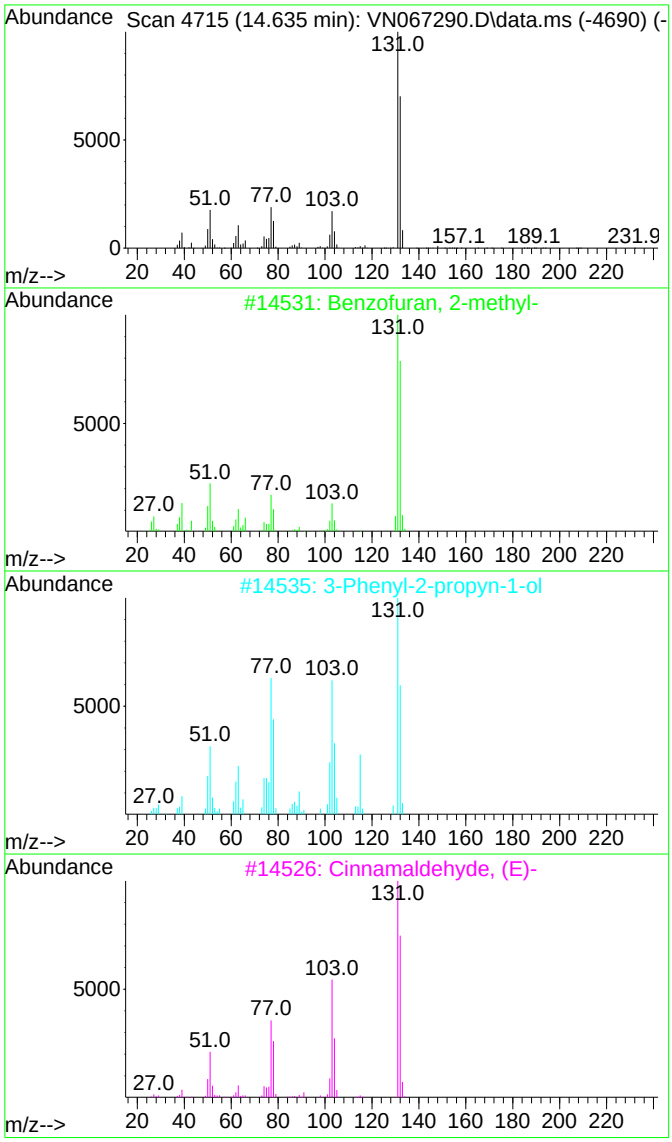
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

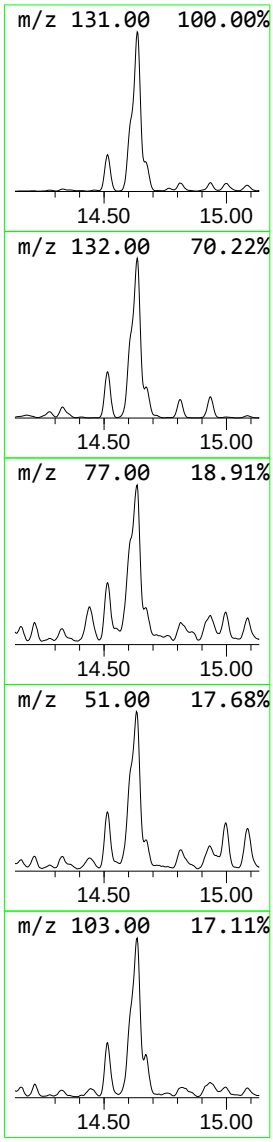
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzofuran, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.635	329.53 ug/l	13233500	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzofuran, 2-methyl-	132	C9H8O	004265-25-2	94
2	3-Phenyl-2-propyn-1-ol	132	C9H8O	001504-58-1	91
3	Cinnamaldehyde, (E)-	132	C9H8O	014371-10-9	90
4	Benzonitrile, 2-(methylamino)-	132	C8H8N2	017583-40-3	87
5	4-Aminobenzyl cyanide	132	C8H8N2	003544-25-0	86





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Acq On : 11 Jun 2021 15:54
Operator : JC/MD
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Misc : 4.91g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-06-060921

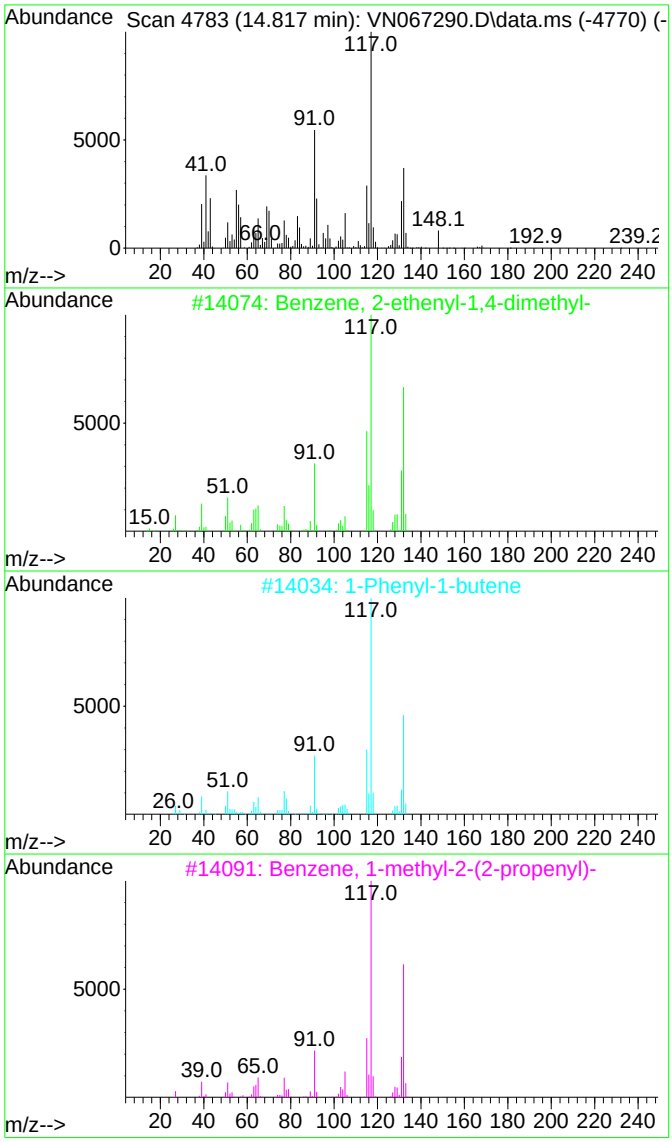
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

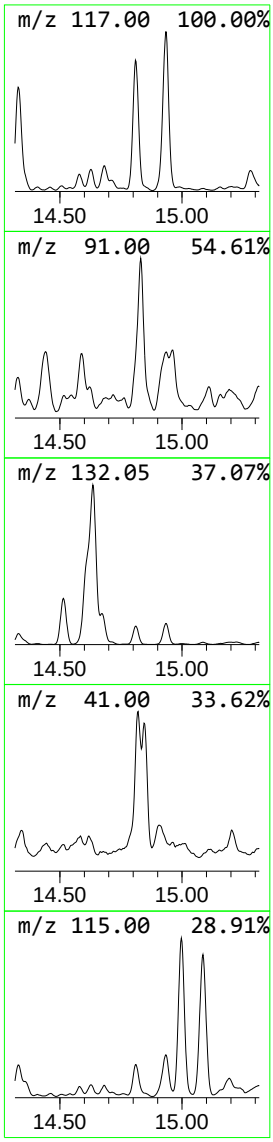
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.817	142.69 ug/l	5730280	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2	1-Phenyl-1-butene	132	C10H12	000824-90-8	93
3	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	70
5	Indan, 1-methyl-	132	C10H12	000767-58-8	70





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Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-06-060921

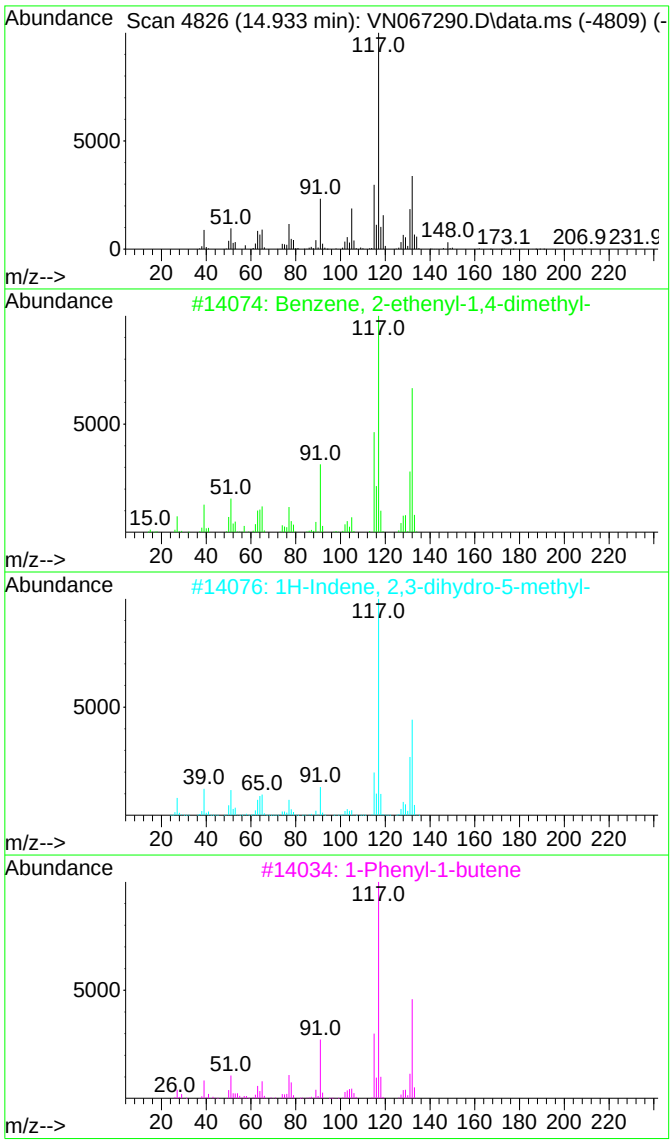
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

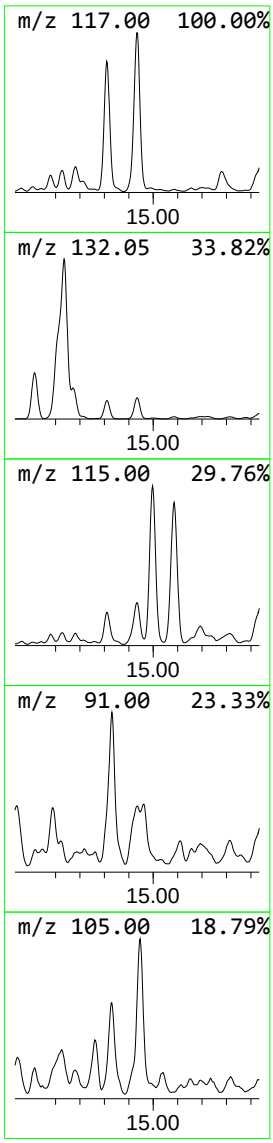
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.933	117.74 ug/l	4728410	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	94
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	94
4	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	93
5	2,4-Dimethylstyrene	132	C10H12	002234-20-0	92





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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

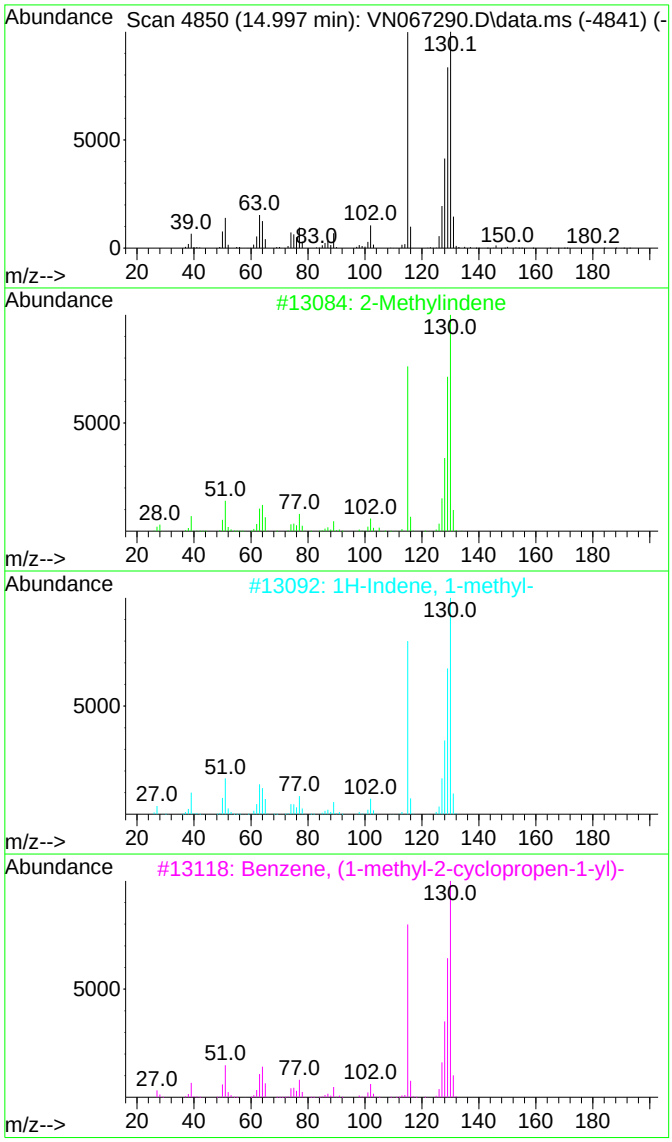
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

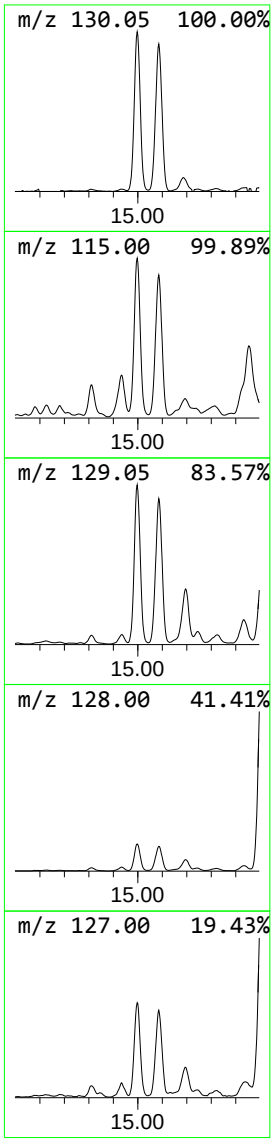
****

Peak Number 6 2-Methylindene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.997	116.06 ug/l	4660880	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylindene	130	C10H10	002177-47-1	97
2	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
3	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	95
4	Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	93
5	1H-Indene, 3-methyl-	130	C10H10	000767-60-2	91





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Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-06-060921

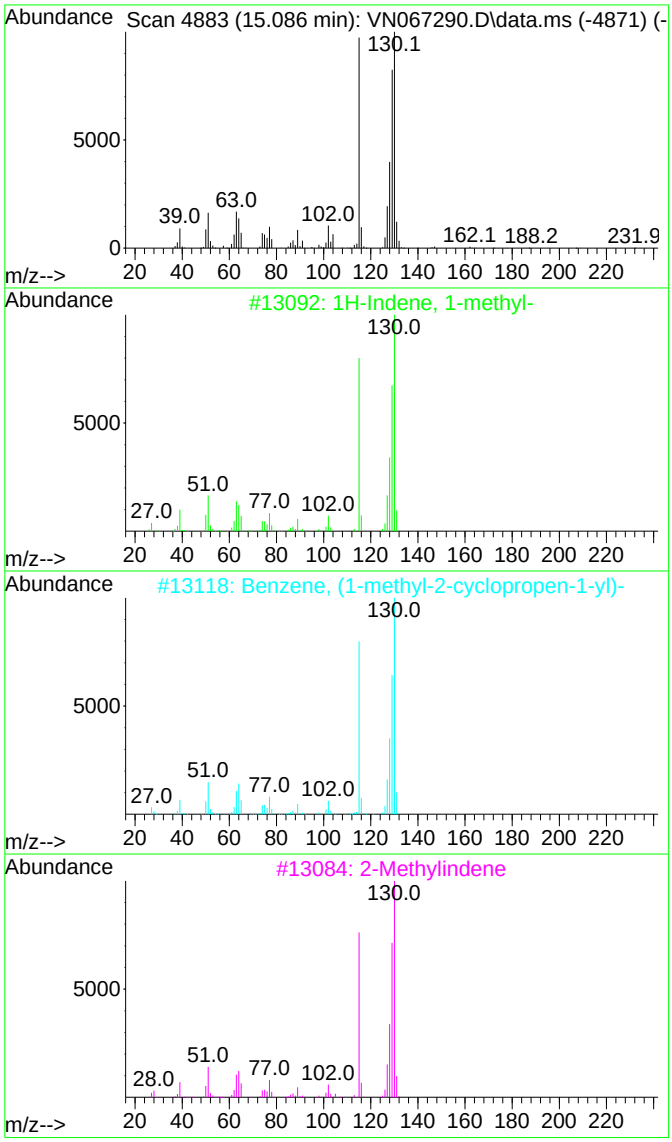
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

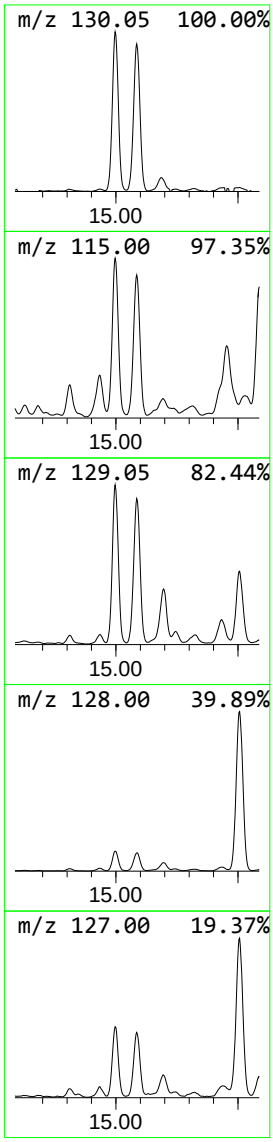
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1H-Indene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.086	105.89 ug/l	4252280	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
2	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	96
3	2-Methylindene	130	C10H10	002177-47-1	96
4	Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	95
5	Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	93





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Instrument :
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ClientSampleId :
TMR-DS-06-060921

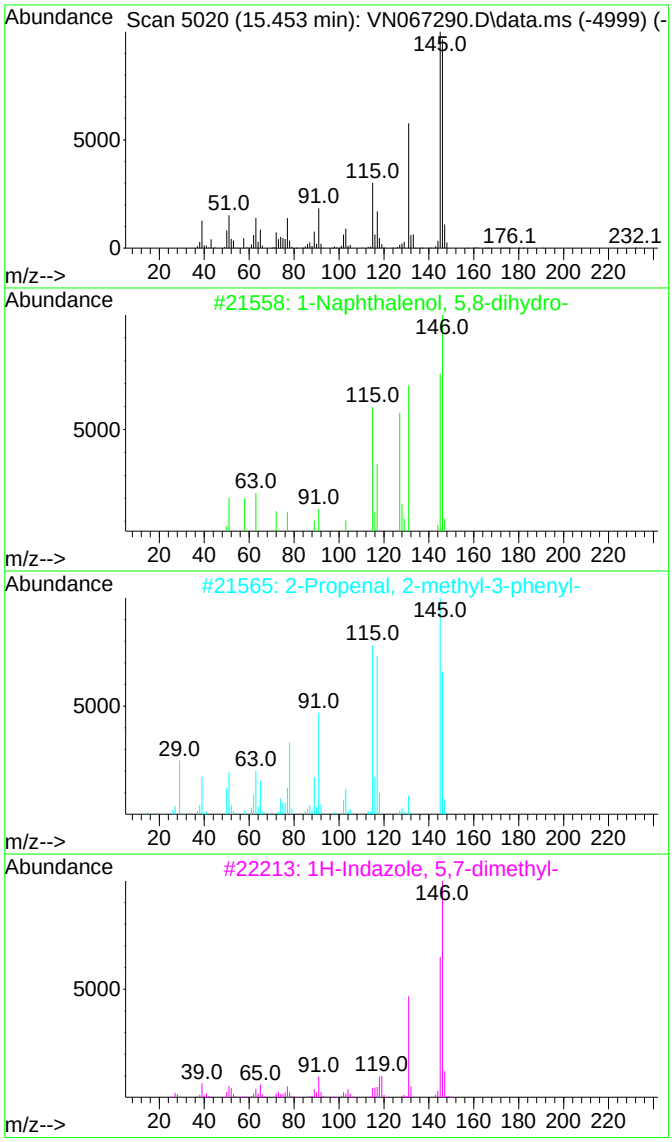
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

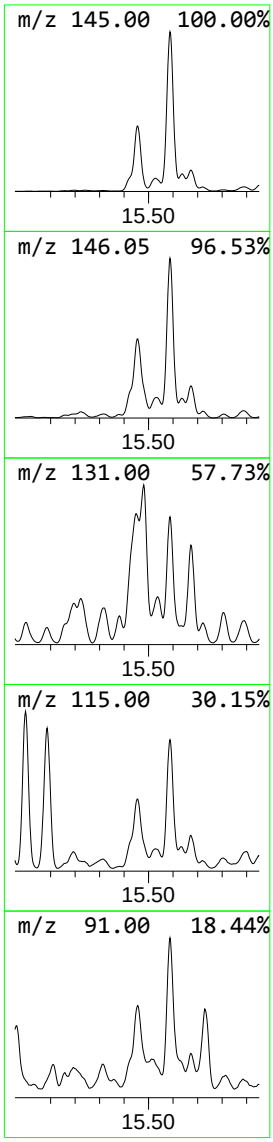
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1-Naphthalenol, 5,8-dihydro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.453	239.04 ug/l	9599570	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Naphthalenol, 5,8-dihydro-	146	C10H10O	027673-48-9	87
2	2-Propenal, 2-methyl-3-phenyl-	146	C10H10O	000101-39-3	76
3	1H-Indazole, 5,7-dimethyl-	146	C9H10N2	043067-41-0	58
4	Benzofuran, 4,7-dimethyl-	146	C10H10O	028715-26-6	53
5	3-Buten-2-one, 4-phenyl-, (E)-	146	C10H10O	001896-62-4	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067290.D
Acq On : 11 Jun 2021 15:54
Operator : JC/MD
Sample : M2674-06 10X
Misc : 4.91g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-06-060921

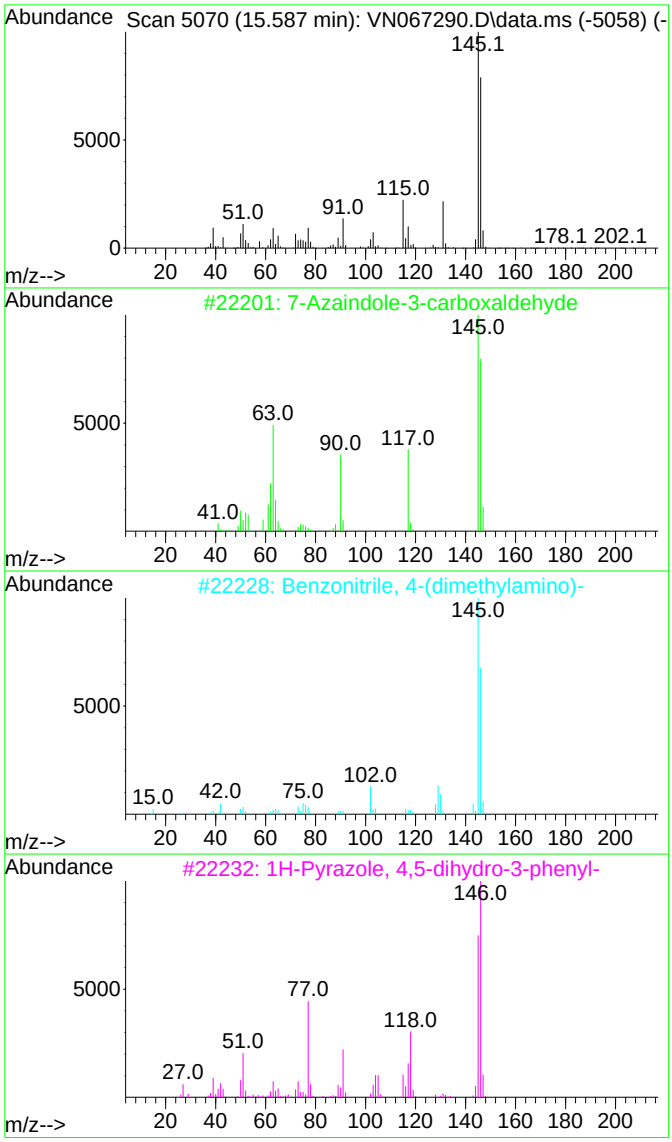
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

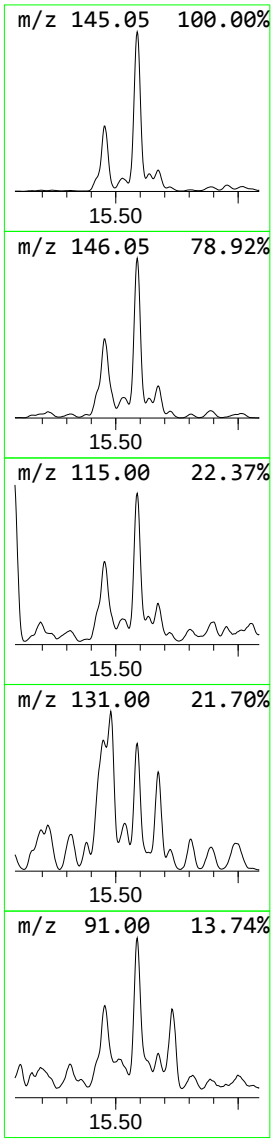
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 7-Azaindole-3-carboxaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.587	288.17 ug/l	11572500	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Azaindole-3-carboxaldehyde	146	C8H6N2O	004649-09-6	59
2	Benzonitrile, 4-(dimethylamino)-	146	C9H10N2	001197-19-9	53
3	1H-Pyrazole, 4,5-dihydro-3-phenyl-	146	C9H10N2	000936-48-1	52
4	Benzofuran, 4,7-dimethyl-	146	C10H10O	028715-26-6	52
5	Cinnoline, 1,2-dihydro-2-methyl-	146	C9H10N2	054063-10-4	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067290.D
Acq On : 11 Jun 2021 15:54
Operator : JC/MD
Sample : M2674-06 10X
Misc : 4.91g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TMR-DS-06-060921

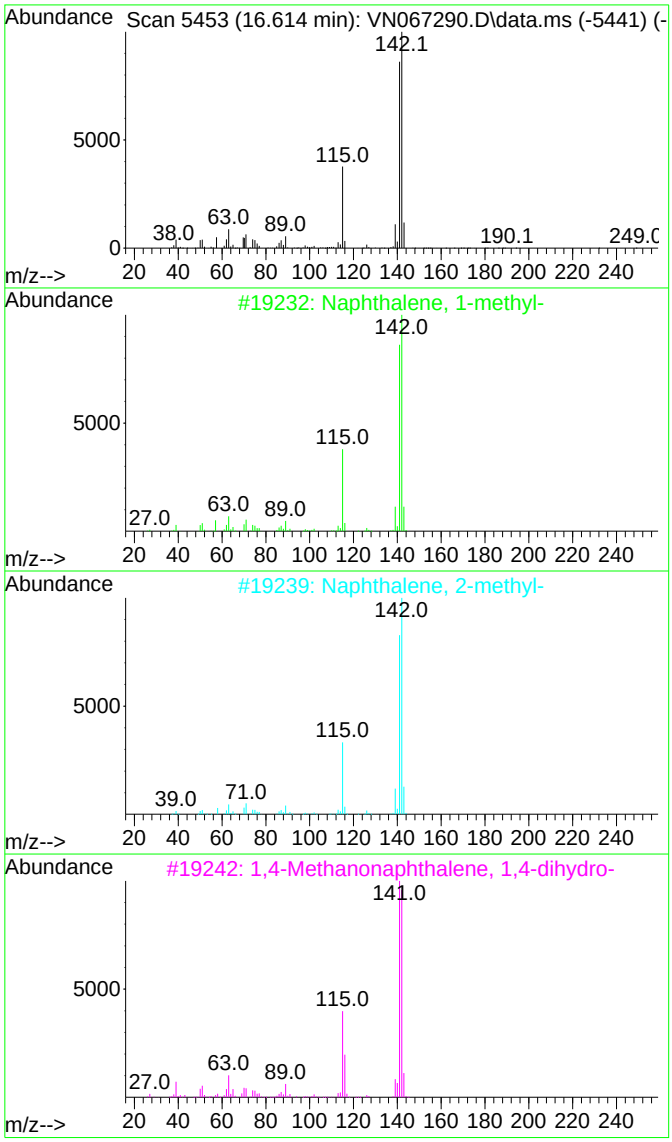
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

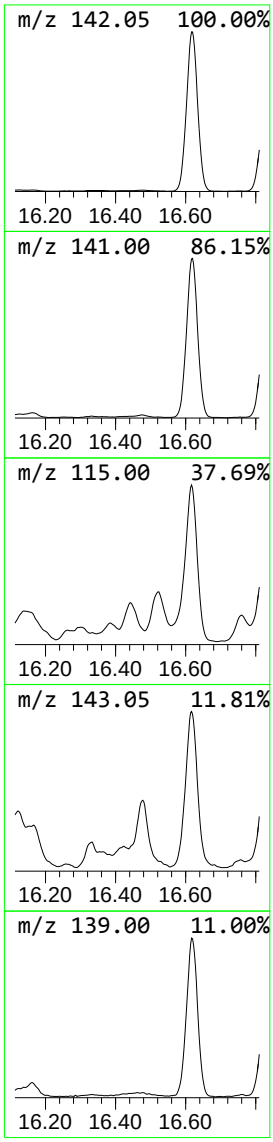
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.614	232.89 ug/l	9352760	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
4	Benzocycloheptatriene	142	C11H10	000264-09-5	90
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
Data File : VN067290.D
Acq On : 11 Jun 2021 15:54
Operator : JC/MD
Sample : M2674-06 10X
Misc : 4.91g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TMR-DS-06-060921

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.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
Benzene, 1-ethy...	12.986	87.4	ug/l	3508910	4	13.675	2007960	50.0
Benzene, 2-prop...	13.873	120.7	ug/l	4848200	4	13.675	2007960	50.0
Benzofuran, 2-m...	14.635	329.5	ug/l	13233500	4	13.675	2007960	50.0
Benzene, 2-ethe...	14.817	142.7	ug/l	5730280	4	13.675	2007960	50.0
1H-Indene, 2,3-...	14.933	117.7	ug/l	4728410	4	13.675	2007960	50.0
2-Methylindene	14.997	116.1	ug/l	4660880	4	13.675	2007960	50.0
1H-Indene, 1-me...	15.086	105.9	ug/l	4252280	4	13.675	2007960	50.0
1-Naphthalenol,...	15.453	239.0	ug/l	9599570	4	13.675	2007960	50.0
7-Azaindole-3-c...	15.587	288.2	ug/l	11572500	4	13.675	2007960	50.0
Naphthalene, 1-...	16.614	232.9	ug/l	9352760	4	13.675	2007960	50.0